Conditions of applicability of the quasiclassical approximation in three-dimensional problems

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Sufficient conditions for the applicability of the quasiclassical approximation in a three-dimensional problem are formulated. The conditions are based on the concept of the Fresnel volume of a classical trajectory; these conditions characterize the "diffraction thickness" of the trajectory and reduce to the requirement that the potential should not change abruptly across the transverse section of the Fresnel volume. A simple method is also proposed for estimating the modulus of the wave function in the caustic regions of inapplicability of the quasiclassical approximation; the method is based on the law of conservation of the probability flux in a tube of trajectories of finite section.

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1. BASIC ASSUMPTIONS

In one-dimensional problems, the condition of applicability of the quasiclassical approximation reduces to the well-known requirement that the de Broglie wavelength $\lambda = h/p = h/[2m(E-U)]^{1/2}$ of a particle with energy E in the potential field $U(x)$ should change little over distances of order λ (Refs. 1–3), i.e., $\lambda[d\lambda/dx] \ll \lambda$ or

$$|d\lambda/dx| \ll 1. \tag{1}$$

In three-dimensional problems, this condition is only necessary but it is not sufficient, since the fulfillment of the inequality (1) by no means guarantees smallness of the diffraction effects, which are not described by the quasiclassical approximation.

Hitherto, the conditions of applicability of the quasiclassical approximation in three-dimensional problems have been obtained only for a number of special cases (see Refs. 1–4 for examples). However, it is possible to formulate general conditions of applicability by requiring that the parameters of the quasiclassical wave function

$$\psi(\mathbf{r}) = A(\mathbf{r})e^{iS(\mathbf{r})/\hbar} \tag{2}$$

(the amplitude A and the momentum components $p_j = \partial S/\partial x_j$) change little within the region important for the formation of the wave function. It is clear that the region of formation is concentrated near the classical trajectory leading to the given point $\mathbf{r}$ (see Fig. 1). Let $2a_f$ be the diameter of the transverse section of this region. Then the general conditions of applicability can be written in the form of the inequalities

$$a_f|\nabla_\perp A| \ll A, \quad a_f|\nabla_\perp p_j| \ll p, \tag{3}$$

which must be satisfied along the complete trajectory (here, $\nabla_\perp$ is the operator of differentiation at right angles to the trajectory). There are at least two ways of deriving the inequality (3) and simultaneously determing the scale a_f. Below, we use the simplest approach, which is based on Hyugens's principle. The calculation of Feynman path integrals by the method of stationary phase leads to the same results.

2. DERIVATION OF THE INEQUALITIES (3) AND ESTIMATE OF a_f

Let ρ' be a radius vector in some plane P, ζ be the distance along the normal to P, $\psi^0(\mathbf{r}') \equiv \psi^0(\rho', \zeta=0)$ be the initial wave function specified on the plane P, and $g(\mathbf{r}, \mathbf{r}')$ be the Green's function of the stationary Schrödinger equation

$$\Delta g + 2m(E-U)\hbar^{-2}g = \delta(\mathbf{r}-\mathbf{r}'). \tag{4}$$

The wave function $\psi(\mathbf{r})$ at an arbitrary point $\mathbf{r}$ can be expressed in terms of its value $\psi^0(\mathbf{r}')$ in the plane P by the diffraction integral

$$\psi(\mathbf{r}) = \frac{1}{2\pi}\int \psi^0(\mathbf{r}')\frac{\partial}{\partial\zeta}g(\mathbf{r}, \mathbf{r}')d^2\rho', \tag{5}$$

which follows from Green's theorem in the case of a flat surface and reflects Hyugens's principle.

The quasiclassical approximation (2) arises from the exact integral representation (5) as a result of calculation of the integral by the method of stationary phase. Therefore, the conditions of applicability of the method of stationary phase are simultaneously the conditions of applicability of the quasiclassical approximation. To apply to the calculation of (5) the method of stationary phase, we represent the initial wave $\psi^0(\mathbf{r}')$ and the Green's function $g(\mathbf{r}, \mathbf{r}')$ in the quasiclassical form:

$$\psi^0(\mathbf{r}') \approx A^0(\mathbf{r}')e^{iS^0(\mathbf{r}')/\hbar}, \quad g(\mathbf{r}, \mathbf{r}') \approx G(\mathbf{r}, \mathbf{r}')e^{iS(\mathbf{r}, \mathbf{r}')/\hbar}, \tag{6}$$

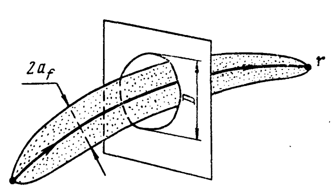

FIG. 1.

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where A^0 and G are the slow (on the scale of the de Broglie wavelength $\lambda = h/p$) amplitude functions. Then by analogy with Ref. 5,

$$\psi(\mathbf{r}') \approx \frac{i}{2\pi\hbar}\int A^0(\mathbf{r}')\frac{\partial S(\mathbf{r},\mathbf{r}')}{\partial\zeta}G(\mathbf{r},\mathbf{r}')e^{i\tilde{S}(\mathbf{r},\mathbf{r}')/\hbar}d^2\rho', \tag{7}$$

$$\tilde{S}(\mathbf{r},\mathbf{r}') = S^0(\mathbf{r}') + S(\mathbf{r},\mathbf{r}').$$

The equation $\nabla'\tilde{S}(\mathbf{r}, \mathbf{r}') = 0$ distinguishes the stationary point $\mathbf{r}'_c = (\rho'_c, 0)$, which serves as the start of the classical trajectory which leads to the point $\mathbf{r}$. The main contribution to the integral (7) is made by the π neighborhood of this point , within which the total phase $\tilde{S}(\mathbf{r}, \mathbf{r}')/\hbar$ differs from its stationary value $\tilde{S}(\mathbf{r}, \mathbf{r}'_c)/\hbar \equiv S(\mathbf{r})/\hbar$ by not more than π, or

$$|\tilde{S}(\mathbf{r},\mathbf{r}') - \tilde{S}(\mathbf{r},\mathbf{r}_c')| \leqslant \pi\hbar = h/2. \tag{8}$$

This equation determines the scale a_f of the region of formation of the wave function $\psi(\mathbf{r})$ in the plane P.

The determination of a_f from Eq. (8) can be significantly simplified by using the fact that a_f is small compared with the length L of the trajectory. This means that in (8) we can make an expansion in the difference $\eta = \mathbf{r}' - \mathbf{r}'_c$ and restrict ourselves in this expansion to the quadratic terms:

$$|\tilde{S}(\mathbf{r},\mathbf{r}') - \tilde{S}(\mathbf{r},\mathbf{r}_c')| \approx {}^1/_2|(\eta\nabla')^2\tilde{S}(\mathbf{r},\mathbf{r}')|_{\mathbf{r}'=\mathbf{r}'_c} = h/2 \tag{9}$$

(the term linear in η is absent because of the extremal properties of the classical trajectory). If the second derivatives vanish, it is necessary to retain in (9) the cubic term, etc.

When the method of stationary phase is used, the pre-exponential factors in (7) are taken outside the integral with their values at the stationary point $\mathbf{r}'_c$. This operation is valid if the pre-exponential factors change little within the π neighborhood of $\mathbf{r}'_c$, and this leads to the inequalitites (3).

In optics, the π neighborhood of the stationary point is called the first Fresnel zone. It is therefore natural to call the set of all the π neighborhoods threaded by the reference trajectory leading to r the Fresnel volume of the classical trajectory of the particle. Above, the Fresnel volume appeared as the region important for the formation of the wave function. It can also be interpreted as the region over which the classical trajectory of the particle is smeared, in the same way that in optics the Fresnel volume characterizes the extent to which the ray trajectory is smeared.[6,7] In principle, the degree of smearing of the trajectory could be determined experimentally by placing a screen with an opening in the path of the flux of particles. Diffraction distortions of the wave function $\psi(r)$ arise when the diameter D of the opening (see Fig. 1) is reduced to $2a_f$.

3. APPLICATIONS

In the various special cases when it is possible to establish the applicability of the quasiclassical approximation (for example, by comparison with an exact or an asymptotic solution), the criteria (3) agree with the already known conditions. Below, we shall use the criteria (3) to determine the caustic region of inapplicability of the quasiclassical approximation and to estimate the wave function in this region.

a) *Estimate of the caustic region of inapplicability of the quasiclassical approximation.* The quasiclassical approximation breaks down near a caustic because the amplitude A becomes infinite. The boundary of the caustic region of inapplicability could be estimated by means of the condition $a_f|\nabla_\perp A| \sim A$, at which the first of the inequalitites (3) is violated, but one can show that in the neighborhood of the caustic this condition is equivalent to the requirement that the π neighborhoods of the stationary points in the integral (7) should touch, i.e., that the difference $|S_1 - S_2|/\hbar$ between the phases along two trajectories leading to the given point r be of order π:

$$|S_1 - S_2| \sim \pi\hbar = h/2. \tag{10}$$

But if n trajectories arrive at the point $\mathbf{r}$, the boundary of the caustic region is determined by the condition that at least two of the many π neighborhoods touch:

$$\min|S_i - S_j| \sim \pi\hbar = h/2, \quad i \neq j, \quad j = 1, 2, \ldots, n. \tag{11}$$

In the case of a simple caustic ($n = 2$), the difference $|S_1 - S_2|$ increases in proportion to $l^{3/2}$, where l is the distance along the normal to the caustic[8,7]:

$$|S_1 - S_2| \approx {}^4/_3 p_c |2\nu|^{1/2} l^{3/2}, \qquad p_c = [2m(E - U_c)]^{1/2}, \tag{12}$$

where $|\nu|$ is the relative curvature of the trajectory and the caustic, and p_c and U_c are the particle momentum and the potential on the caustic. Substituting (12) in (10), we obtain the following estimate for the width of the caustic region of inapplicability:

$$l_c = 1.77\Lambda, \quad \Lambda = (\hbar^2/2p_c^2|\nu|)^{1/3}. \tag{13}$$

This result agrees well with the local Airy asymptotic behavior of the wave function.[8,9] Indeed, the maximum of the Airy function is separated from the caustic by the distance $l' = 1.02\Lambda$, and the first zero by the distance $l'' = 2.34\Lambda$, so that our estimate of l_c lies between l' and l''. For estimates, it is convenient to take as the measure of the width of the caustic region the characteristic scale $\Lambda = (\hbar^2/2p_c^2|\nu|)^{1/3}$.

b) *Estimate of the wave function in the neighborhood of a caustic.* Although the quasiclassical approximation breaks down in the immediate proximity of a caustic, it can be used to obtain the correct order of magnitude of $|\psi|^2$ by applying the quasiclassical law of conservation of the probability flux in a pencil of classical trajectories to the caustic region, the wave function being assumed to be uniformly "smeared" over this region. Then an estimate of the wave function on the caustic, $|\psi_c|$, can be taken to be the averaged quantity

$$|\overline{\psi_c}| = |\psi^0|(p^0\Sigma^0/p_c\Sigma_c)^{1/2}, \tag{14}$$

where Σ_c is the transverse section of the pencil of trajectories corresponding to the caustic region, and Σ^0 is the initial transverse section of this pencil.

Comparison with the results of exact[10] and asymptotic (Ref. 1, Sec. 127, and Ref. 4) calculations shows that in the case of a simple caustic formed by scattering on a centrally symmetric potential formula (14) gives (for width Λ of the caustic region) a value of $|\bar{\Psi}_c|$ which differs from the value $|\psi_{1m}|$ at the first maximum of the Airy function by a coefficient 0.80, i.e., a value only 20% smaller. Bearing in mind that $|\bar{\Psi}_c|$ is an estimate of the wave function averaged over the caustic region, the difference is even less. Considering also the analogous results for electromagnetic and acoustic waves,[6,7] it is to be expected that for the more complicated caustics as well the estimate (14) will give an error not exceeding 20–50%.

4. GENERALIZATIONS

The estimates proposed above admit generalizations in several directions. First, inequalities of the type (3) can be extended to the case of nonstationary problems by introducing the concept of a Fresnel volume in space-time, as in analogous electrodynamic problems.[6,7] Second, the conditions (3) can be readily extended to vector problems of quantum mechanics. In this case, it is necessary to impose the requirement of small changes in the spin state within the Fresnel volume. Third, the arguments presented here can be used to analyze the applicability of the asymptotic methods (the comparison function method[4,11-13] and Maslov's canonical operator method[13,14,15]), which eliminate the principal shortcoming of the quasiclassical approximation, namely the divergence on the caustics.

Finally, it is possible that the prescriptions introduced here for determining the Fresnel volume will simplify the finding of the regions which are important for integration in a function space.

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