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Regularization of Quantum Tunneling of Singular Potential Barrier

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Abstract—The quantum tunneling of a singular potential is modeled, as a rule, by the method of regularization. It proceeds from the intermediate usage of a nonsingular-type preimage of the potential function. In this work, it has been ascertained that the preimages continuously differentiable at the point of singularity does not reproduce the singularity in the problem of quantum tunneling.

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1. INTRODUCTION

In quantum mechanics, the singular potentials $V(x) \sim x^{-\alpha}$, $\alpha > 0$ are of independent interest, simplistically modeling the localized contact interactions [1–3] (note that this includes both the Coulomb and gravitational potentials). Of interest is the case of quantum tunneling [4, 5], when the singularity point $x = 0$ should be passed. As a number of authors indicate [6, 7], there is no single answer to the solution of this problem so far. True, the requirement of continuity of the probability stream for the class of potentials $V(x) \sim x^{-\alpha}$ ($0 < \alpha < 2$) meets no objections, but a purely mathematical analysis of the situation on the basis of a self-adjoint extension of the operators used shows that this continuity is not enough for an unambiguous statement of the problem [8–10]. Additional considerations are required (preferably of a physical plan). The most usual is the method of regularization [11–14]. There, the singular form of the potential function is temporarily replaced by a nonsingular inverse image that provides an analytical solution to the problem. Finally, already in the expressions of the transmission coefficient and reflection coefficient, a passage to the limit is made to restore the infinitely large value of the potential at the singular point $x = 0$.

To clarify the essence of the problem using a simple example, the case of the Dirac delta potential of a certain ‘power’ was considered in [15], when the approach to the solving of the particle-tunneling problem is well known, but the situation differs from the standard one. In the general case, this potential is partially permeable for passage and can be modeled from the problem of the rectangular potential by the limiting narrowing of the area of action under condition that the ‘area’ of the graph tends to the value of the ‘power’ g. That is, the intermediate choice of a rectangular shape with the subsequent passage to the limit of the indicated type is the regularization for the Dirac delta potential.

Unfortunately, not everything is so coordinated in the general case of singular potentials. This primarily refers to the fact that the ‘area’ under the potential graph is an unlimited quantity, stretched over an infinite length. The second, that the derivative of the potential function diverges modulo with the approaching the point $x = 0$, but is not defined, similarly as the potential itself, at the point. Under these conditions, the question arises as to whether there are restrictions on the properties of the functions chosen for the implementation procedure. To answer this question, one must first determine the asymptotic properties of the transmission coefficient of the potential barrier, determined on the basis of the intermediate potential function. A rectangular type of the potential enables such an opportunity, providing the regularization of the tunneling of the Dirac delta potential.

2. ASYMPTOTIC QUANTUM TUNNELING OF THE RECTANGULAR POTENTIAL BARRIER

As is known from the textbooks of quantum mechanics (see, for example, [16]), the transmission coefficient of the rectangular potential barrier is given by the expression

$$T = \frac{1}{1 + \dfrac{V^2}{4E\left|V-E\right|}\mathrm{sh}^2\left(\sqrt{2m\left(V-E\right)}\,a/\hbar\right)}, \tag{1}$$

where E and m are the particle energy and mass, V and a are the width and height of the potential. Two limit transitions are trivial and hold to be true for any regular potential:

$$T \xrightarrow[E=const]{V\to\infty} 0, \quad T \xrightarrow[V=const]{E\to\infty} 1. \tag{2}$$

Therefore, they cannot serve as tests for choosing the intermediate type of potential of the regularization method.

When the energy of the particle and the height of the barrier simultaneously tend to infinity, remaining all the time equal or equidistant, another limit is as follows

$$T \xrightarrow[E-V=const]{V\to\infty,\, E\to\infty} 0. \tag{3}$$

The last limit that reproduces the result of the delta potential:

$$T \xrightarrow[Va=g,\, E=const]{V\to\infty,\, a\to 0} \left(1 + \frac{g^2 m}{2\hbar^2 E}\right)^{-1}. \tag{4}$$

The answer depends on the 'power' $g = Va$ of the barrier.

3. ASYMPTOTIC QUANTUM TUNNELING OF A POTENTIAL BARRIER WITH A SMOOTH TOP

Consider the asymptotic laws of tunneling of a smoothly varying potential with a peak at the point $x = 0$. Once again we turn to the example known from textbooks (see, for example, [16]), to the bell-shaped potential $V\left(x\right) = V_0 / \mathrm{ch}^2\alpha x$. The transmission coefficient is given by the expression

$$T = \frac{\mathrm{sh}^2 \dfrac{\pi k}{\alpha}}{\mathrm{sh}^2 \dfrac{\pi k}{\alpha} + \mathrm{ch}^2\left(\dfrac{\pi}{2}\sqrt{\dfrac{8mV_0}{\hbar^2\alpha^2} - 1}\right)}. \tag{5}$$

By a direct computation it is easy to verify that a limit similar to (3) is not zero, but equal to 1/2:

$$T \xrightarrow[E-V_0=const]{V_0\to\infty,\, E\to\infty} 1/2. \tag{6}$$

The last limit – the contraction of the potential curve into the line while conserving the 'power' $g = 2V_0 / \alpha$ exactly reproduces (4).

The coincidence of the limiting form (4) for the chosen two forms shows that the property of the delta function to be represented by the limiting restriction of any function of the given area under the curve extends also to the corresponding solutions of the Schrödinger equation. In other words, the analytical solution to the Schrödinger equation for the Dirac delta potential is self-consistent with the regularized solutions. This can be interpreted also as a direct consequence of the fact that the Dirac delta function is not a function, among them a singular function, in the classical sense, but a continuous linear functional on the space of differentiable functions.

The other conclusion is important for us that the rectangular and bell-shaped forms have at least one different asymptotic limit. Since the distinction is numerical, and independent on the potential parameters, the limits (3) and (6) reveal the existing immanent and qualitative difference between these functions. Naturally, it consists in the behavior of the derivative of a potential function in a neighborhood of a point in the course of the limiting approaching to the singular form [15].

Before continuing the discussion, let us find out how general is the distinctive limiting result (6) for potentials with the smooth character of maximum. For this, let us consider the parabolic form of the potential different from the bell-shaped:

$$V(x) = V_0\left(1 - \frac{x^2}{a^2}\right), \quad -a \le x \le a . \tag{7}$$

Linearly independent wave functions outside the region of potential are traveling waves, and in the potential region they are expressed in terms of the functions of a parabolic cylinder $D_\nu(\lambda z)$:

$$\psi(z) = B_1 D_\nu\left(\left(1+\mathrm{i}\right)u_0^{1/4} z\right) + B_2 D_{\nu^*}\left(\left(-1+\mathrm{i}\right)u_0^{1/4} z\right), \tag{8}$$

where $\nu = -1/2 - \mathrm{i}\,\varepsilon/\sqrt{u_0} + \mathrm{i}\sqrt{u_0}/2$. The particle energy ε and barrier height u_0 are normalized to the energy $E_r = \hbar^2 / 2ma^2$. The rest of the calculations are carried out in a standard way and for the transmission coefficient they give an asymptotic value of 1/2, which exactly coincides with the value (6) of the bell-shaped barrier. Therefore, one can conclude that if the potential function of the barrier is continuously differentiable near the peak, then the asymptotic limit (6) takes place. The course of transmission and reflection coefficients to half value is shown in Fig. 1. Note that the assumption of the presence of such specifics was made in [15].

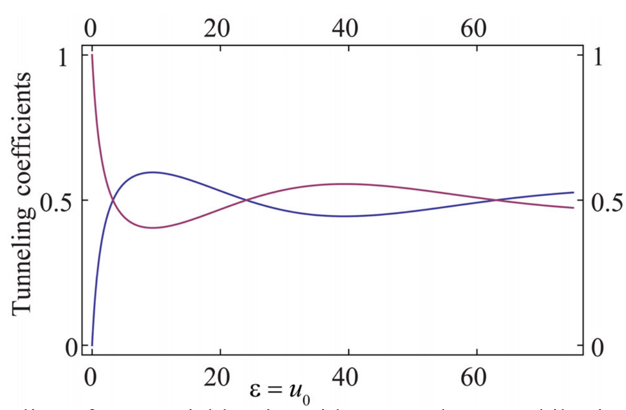

Fig. 1. The quantum tunneling of a potential barrier with a smooth apex while simultaneously increasing the height of the barrier u_0 and the energy ε of the particle incident on the barrier. The reflection coefficient graph starts from zero, the transmission coefficient starts from unity.

4. ASYMPTOTIC QUANTUM TUNNELING OF A SHARP-PEAK POTENTIAL BARRIER

In fact, the condition of continuous differentiability for the limit (6) is not only sufficient, but also a necessary condition. To verify this, let us consider a potential with a sharp peak whose wings drop to zero at points $x = \pm a$ according to, for example, the parabolic law:

$$V(x) = V_0\left(1 - \frac{x}{a}\operatorname{sign}x\right)^2, \quad -a \le x \le a. \tag{9}$$

The wave function in the range of potential:

$$\psi(z) = B_1 D_\nu\left(-\sqrt{2}\,u_0^{1/4}(1-z)\right) + B_2 D_\nu\left(-\mathrm{i}\sqrt{2}\,u_0^{1/4}(1-z)\right),$$

where $\nu = -\left(\varepsilon + \sqrt{u_0}\right)/2\sqrt{u_0}$. Then, the reflection and transmission coefficients can be computed analytically to the end, as in the previous case. Substituting the condition and infinitely increasing the barrier height, we obtain the asymptotic values different from 1/2 for the reflection and transmission coefficients. The graphs of approximation to the asymptotic values are represented in Fig. 2.

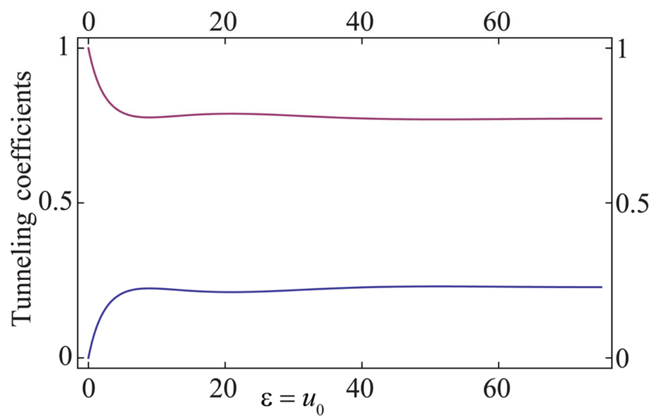

Fig. 2. The quantum tunneling of a potential barrier with a smooth apex while simultaneously increasing the height of the barrier u_0 and the energy ε of the particle incident on the barrier u_0. The reflection coefficient graph starts from zero, the transmission coefficient starts from unity.

Thus, the asymptotic behavior of the reflection and transmission coefficients in a special case $\varepsilon = u_0 \to \infty$ uniquely depends on the nature of the potential function near the maximum.

If it is continuously differentiable, that is, it has a certain derivative at the maximum point, and then the boundary values of the reflection and transmission coefficients are equal to each other. If the maximum is sharp, that is, the derivative of the potential curve does not have a certain value at the maximum point, and then the boundary value of the reflection coefficient is less than the transmission coefficient. This remarkable property can be used in the process of regularization of singular potentials. Indeed, the fact that the special limit with a smooth peak of the potential is half, but with a sharp peak is not, suggests that these potential functions, and hence their limits, differ in essential feature. For the limiting types of potentials, only a singularity can be such. Because the potential functions with a sharp vertex in the limit of infinite height really reproduce the properties of singular functions, this cannot be said for the smooth vertices of functions. Therefore, the potential functions with a continuously defined derivative near the maximum cannot be chosen as the prototypes for performing the intermediate computations in the regularization method of singular potentials. This class of functions in the limit obtains an infinitely large value at the point $x = 0$ but does not become singular.

5. CONCLUSION

The singular potentials constitute a separate class in the problems of physics, and in particular – of quantum mechanics. Because of the lack of the immediate mathematical conditions for the binding of solutions on both sides of the point of divergence of potential, the additional physical assumptions is to be made to consider the problem of quantum tunneling. In practice, it comes to the regularization method, when the singular potential is replaced preliminarily by a prototype potential of finite height. The problem is analytically solved for this potential, and finally, in these solutions including the reflection and transmission coefficients, the height of the potential at a singular point of the initial potential tends to infinity.

Thus, it is shown that the character of the solutions inherent to the singularity in the interaction potential can be restored by the regularization method, unless the prototype function has a definite derivative at the singularity point of the initial potential.

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