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On Quantum Tunneling of a Singular Potential

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Abstract—To get around the difficulty that the singular nature of the potential function $V(x) = V_0/|x|^\alpha$ introduces into physics, the regularization methods are used. However, they affect the singular nature of the problem, and so we discuss here how quantum tunneling behaves if the original singular nature of the Schrodinger equation remains unperturbed. For this purpose, I am starting from the precondition that the singular terms are mutually compensated in the current probability density and the current can be considered continuous. As a result, it is obtained that the mild-singular potential (with $0 < \alpha < 1$) has finite but unusual tunnel transparency, in particular, a non-zero value at zero energy of the incident particle. The transparency of a Coulomb potential well oscillates infinitely at zero energy, and only the strongly singular potential (with $\alpha > 1$) repeats the property of the regularized prototypes: to be impenetrable.

Keywords: quantum tunneling, singular potential, 1D Coulomb potential
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1. INTRODUCTION

A fundamental feature of the singular potential [1–3] is the absence of a singularity point in the region of a potential energy function. At the same time, quantum tunneling implies a transition through the singularity point and, therefore, some rules for this transition. For this, the potential cutoff method is used, or the conditions for matching the wave function and its derivative on both sides of the singular point are introduced. The first method replaces the singular form with a regular one with a cutoff singular part, for which the transmittance and reflection coefficients are computed, and then a passage to the limit is made in the expressions for these coefficients, narrowing the cutoff width to zero [4–7]. And the second method, based on the matching conditions, requires the representation of physical quantities by the Hermitian operators [8–11]. Thus, claiming the existence of the quantum-mechanical average of the singular potential energy, in [12] the singularity is divided into three classes: moderate, intermediate, and super-singular class. In terms of the potential function $V(x) = V_0/|x|^\alpha$, they correspond to the parameter ranges of $0 < \alpha < 1$, $1 \le \alpha < 2$, and $\alpha \ge 2$, respectively. It is noted that for a moderate singular class, both solutions are regular and, in principle, can be admitted to the tunneling problem. For an intermediate singular class, only one solution is regular and, therefore, acceptable in the procedure for solving a physical problem. In the supersingular case, both solutions diverge.

The greatest attention was paid to the tunneling of the 1D Coulomb potential. Restricting only to regular solutions automatically results in the absence of a probabilistic current and, consequently, to the impenetrability of the potential barrier. This result was also obtained by the method of limiting smoothing of the potential barrier [12] and later confirmed in a short presentation [13]. Further, considering the antisymmetric potential distribution [14], the irregular solution of the problem was transformed into a regular one by a certain procedure that results in the finite permittivity of the antisymmetric Coulomb potential. In [15], this approach is called ingenious but justified not entirely. The answer [16] substantiates that this criticism refers to the symmetric and not to the antisymmetric form of the potential distribution, which was considered there.

In [17], the problem of tunneling the Coulomb potential is considered from the point of view of the analytical continuation of solutions through the singularity point in combination with the method of varying constants. This allows one to completely solve the problem of 1D tunneling and get any permeability other than total: one just needs to select the appropriate type of self-adjoint expansion. In [18], the permeability problem was revised based on self-adjoint extensions and it was determined that the important

Dirichlet boundary condition implies an impenetrable origin of coordinates. Finally, the approach [19], by analogy with [14], removes the singularity of the wave function, but at the same time results in zero permeability for the singular center of the potential.

Besides the Coulomb tunneling, quantum tunneling has also been studied for the inverse quadratic potential $V(x) = V_0/|x|^2$. In [20], the transmission coefficient was determined for all possible self-adjoint extensions of the Hamiltonian with the condition $0 < V_0 < 3/4$ and it was established that tunneling is possible and it occurs if the matrix of self-adjoint extensions is not diagonal. The possibility of tunneling under the same conditions is also asserted based on the family of nonequivalent $U(2)$ quantization [21].

Note, however, that the indicated regularization procedures, introduced to reconcile the Schrödinger equation with the standard postulates of quantum mechanics, suppress to some extent the original content of the singular problem. For this reason, here I study the problem of what is the quantum tunneling of a singular potential in the framework of the Schrödinger equation but without any action to strictly comply with the postulates of quantum mechanics. The approach used is based on the property of the current density of the probability that the singular terms in it balance each other, and therefore the continuity of the current can be extended to the entire coordinate axis, including the singular origin of coordinates. This approach was previously applied to the case of a 1D Coulomb potential barrier ($\alpha = 1, V_0 > 0$) in [22]. The present consideration includes moderate- ($0 < \alpha < 1$), intermediate- ($1 < \alpha < 2$), super- ($\alpha \geq 2$) singular ranges, and the 1D Coulomb well ($\alpha = 1, V_0 < 0$), thus, together with [22], it covers all ranges of parameters $\alpha > 0$ and V_0.

2. STATEMENT OF THE PROBLEM

The stationary Schrödinger equation for the singular potential has the form

$$\frac{d^2\psi(z)}{dz^2} + \left(\varepsilon - \frac{u_0}{|z|^\alpha}\right)\psi(z) = 0, \tag{1}$$

where z is normalized to an arbitrary length l, and the energy of the particle and the 'power' of the potential—to the "recoil energy" $E_{\text{rec}} = \hbar^2/2ml^2$. We will seek the solution in the form

$$\psi(z) = \exp\left(h(z) \pm i\sqrt{\varepsilon}\, z\right) \tag{2}$$

with an unknown function $h(z)$, which, according to (1), must satisfy the equation,

$$h''(z) + (h'(z))^2 \pm i\,2\sqrt{\varepsilon}h'(z) = u_0|z|^{-\alpha} \tag{3}$$

and the derivative of which must disappear at infinity. Equation (3) for general non-integer values of the degree does not have exact solutions expressed in known analytical functions. In what follows, we construct approximate solutions while preserving the singular nature of the equation (3).

3. QUANTUM TUNNELING OF MODERATELY SINGULAR POTENTIAL

The leading-order contributions on the right and left sides of Eq. (3) near the singular point must be of the same order of magnitude, so we have

$$h''(z) \overset{z\to 0}{\approx} u_0|z|^{-\alpha} \tag{4}$$

and correspondingly

$$h'(z) \overset{z\to 0}{\approx} \frac{u_0}{1-\alpha}|z|^{1-\alpha}. \tag{5}$$

Because $0 < \alpha < 1$ we have

$$(h'(z))^2 \ll h'(z) \tag{6}$$

and this term can be omitted in equation (3). Then it takes the form

$$h''(z) \pm i\,2\sqrt{\varepsilon}h'(z) = u_0|z|^{-\alpha}. \tag{7}$$

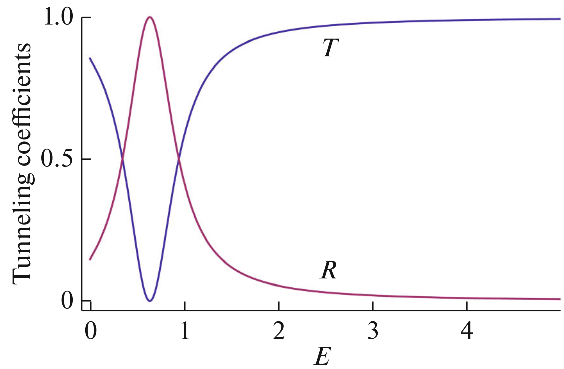

Fig. 1. Transmission and reflection coefficients of a moderately singular potential barrier depending on the energy of incident particles for $u_0 = 1$, $\alpha = 0.25$. The appearance of total reflection and nonzero transmission at zero energy is caused by the singular character of the potential function.

It should be noted that although condition (6) is gradually violated with distance from the origin of coordinates because the tunneling problem will be formulated by values at the origin of coordinates, it is only important that at large distances $h'(z)$ is proportional to $|z|^{-\alpha}$ and, accordingly, the solution of equation (7) satisfies the necessary condition for vanishing at infinity. Equation (7) is of the first order for the derivative $h'(z)$, and its solution for the coordinates $z > 0$ has the form

$$h'(z) = -e^{\mp i\times 2\sqrt{\varepsilon}z} z^{1-\alpha} \left(\mp i\, 2\sqrt{\varepsilon}z\right)^{-1+\alpha} \Gamma(1-\alpha, \mp i\times 2\sqrt{\varepsilon}z)\, u_0, \tag{8}$$

where the constant of integration is taken equal to zero to provide a zero solution in the absence of potential ($u_0 = 0$). By direct integration of (8), we obtain

$$h(z) = -\frac{2^{-2+\alpha}(\mp i\sqrt{\varepsilon})^{\alpha}}{\varepsilon}\left(\frac{\pi\csc(\pi\alpha)}{\Gamma(\alpha)} \pm \frac{i\, e^{\mp i\times 2\sqrt{\varepsilon}z}\Gamma(2-\alpha, \mp i\, 2\sqrt{\varepsilon}z)}{1-\alpha}\right)u_0. \tag{9}$$

Similarly, on the left side of the potential for the desired function, we obtain

$$h'(z) = \mp\frac{i}{2} e^{\mp i\times 2\sqrt{\varepsilon}z} (\pm 2i)^{\alpha} \varepsilon^{(-1+\alpha)/2} \Gamma(1-\alpha, \mp i\times 2\sqrt{\varepsilon}z)\, u_0, \tag{10}$$

$$h(z) = -(\pm i)^{1+\alpha}(2\sqrt{\varepsilon})^{-1+\alpha}\left(\frac{2^{-\alpha} z(\mp i\sqrt{\varepsilon}z)^{-\alpha}}{-1+\alpha} \pm \frac{i\left(\Gamma(1-\alpha)\right) - e^{\mp i\times 2\sqrt{\varepsilon}z}\Gamma(1-\alpha, \mp i\, 2\sqrt{\varepsilon}z)}{2\sqrt{\varepsilon}}\right)u_0. \tag{11}$$

The use of expressions (8)–(11) shows that linearly independent solutions (2) and their derivatives are finite at a singular point $z = 0$. Therefore, the continuity conditions can be applied to the general solution of the problem under consideration. Then, assuming the asymptotic absence of a wave propagating to the right on the right side of the potential we, obtain the following explicit expressions for the normalized amplitudes of the transmitted and reflected waves:

$$t = \frac{2\varepsilon - (2i)^{\alpha}\varepsilon^{\alpha/2}\Gamma(1-\alpha)u_0}{2\left(2\varepsilon - (-2i)^{\alpha}\varepsilon^{\alpha/2}\Gamma(1-\alpha)u_0\right)} + \frac{1}{2}, \tag{12}$$

$$r = \frac{2\varepsilon - (2i)^{\alpha}\varepsilon^{\alpha/2}\Gamma(1-\alpha)u_0}{2\left(2\varepsilon - (-2i)^{\alpha}\varepsilon^{\alpha/2}\Gamma(1-\alpha)u_0\right)} - \frac{1}{2}. \tag{13}$$

Figure 1 shows the graphs of the dependence of the transmittance $T = |t|^2$ and the reflection coefficient $R = |r|^2$ on the energy of the incident particle for the potential barrier ($u_0 > 0$). The case of a potential well ($u_0 < 0$) is illustrated in Fig. 2. It can be seen that quantum tunneling exhibits unusual behavior in the low and moderate energy ranges: the probability of crossing the singular point starts from a nonzero value, and in the case of a potential barrier, the reflection coefficient for some incident energy increases

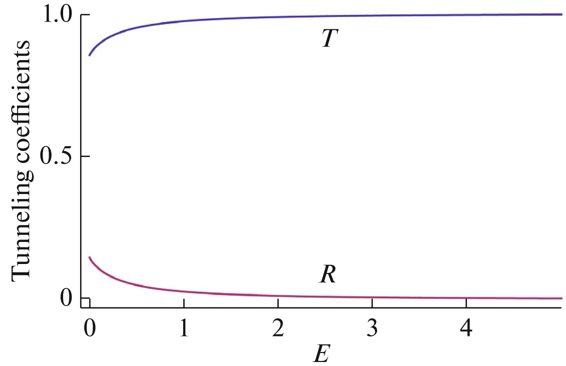

Fig. 2. Transmittance and reflection coefficients of a moderately singular potential well as a function of the energy of incident particles for $u_0 = -1$. An unusual feature here is the nonzero transparency in the zero energy limit. Parameter α has the same meaning as in Fig. 1.

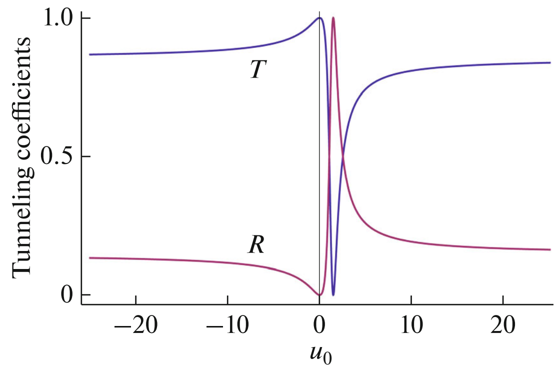

Fig. 3. Quantum tunneling coefficients of a moderately singular potential as a function of power u_0 at $\varepsilon = 1$.

to unity, which is by no means typical for a separate regular potential barrier [23, 24]. The natural law here is the ascent to full transparency at asymptotically high energies. The dependence on the power of the potential is also unnatural (Fig. 3).

4. QUANTUM TUNNELING OF A 1D COULOMB POTENTIAL WELL

For this potential $u_0 < 0$ and $\alpha = 1$, and the Schrödinger equation (1) outside the singular point has an exact analytical solution. To avoid repetition, let us only say that they are identical to the formulas presented in [22], implying that $u_0 < 0$ there. It is important here that one of the linearly independent solutions, together with its derivative, is regular. Another solution is also regular, but its derivative diverges logarithmically as it approaches the singular point. The first gives us the right to refer to the postulate of the continuity of the wave function all over the space, including the singular origin. However, the continuity of the derivative of the wave function at the singularity point does not in any way follow from the Schrödinger equation for the considered Coulomb potential. Therefore, this condition, which is familiar to regular potentials, must be replaced by a new one. The density of probability flow seems to be the most appropriate here because the singular behavior of the terms is mutually suppressed in this expression. Then, after the standard procedure for setting and computing the tunneling problem, it turns out to be possible to unambiguously derive the expressions for the transmission and reflection coefficients [22].

The tunneling efficiency shown in Fig. 4, oscillates between zero and one, and the frequency of oscillations increases to infinity as it approaches the zero boundary of the particle's energy. At the high-energy limit, the probability of quantum transmission (reflection) vanishes monotonically (becomes complete) [22]: tunneling of the 1D Coulomb well behaves similarly to tunneling of the Coulomb barrier.

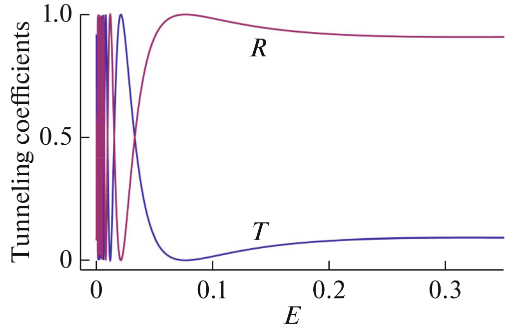

Fig. 4. Coefficients T and R for the 1D Coulomb potential depending on the energy of the incident particle at $u_0 = -1$. Unusual features are infinitely accelerating oscillations in the zero-energy limit and the approach of T (R) to zero (unity) in the high-energy limit. The decreasing of $|u_0|$ slows down the oscillation frequency.

5. QUANTUM TUNNELING OF INTERMEDIATE SINGULAR POTENTIAL

Near the origin of coordinates, asymptotic formulas (4) and (5) remain valid, from which it follows

$$h(z) \approx \frac{u_0}{(1-\alpha)(2-\alpha)} |z|^{2-\alpha} \underset{z\to 0}{\longrightarrow} 0. \tag{14}$$

This, according to equation (2), gives the boundary condition $\psi(z) \underset{z\to 0}{\longrightarrow} 1$, which means that in the limit $z \to 0$ both basic solutions of the Schrödinger equation are finite. Then, without loss of generality, we can assume the continuity of the general wave function, which is written in the form of the following condition:

$$a_{l,\text{plus}} + a_{l,\text{minus}} = a_{r,\text{plus}} + a_{r,\text{minus}}, \tag{15}$$

where $a_{l(r),\text{plus}}$ and $a_{l(r),\text{minus}}$ are amplitudes of probabilities in the general wave function, respectively, before the basis solutions $\psi_{l(r),\text{plus}}(z)$ and $\psi_{l(r),\text{minus}}(z)$ equation (7) to the left (right) of the singular point of the potential. The absence of the reflected wave in the asymptotics $z \to +\infty$ implies the condition $a_{r,\text{minus}} = 0$, and then the continuity condition (15) takes the simpler form:

$$a_{l,\text{plus}} + a_{l,\text{minus}} = a_{r,\text{plus}}. \tag{16}$$

At a large distance, the probability current density is reduced to the expression

$$i\kappa\left(|a_{l,\text{minus}}|^2 - |a_{l,\text{plus}}|^2\right)\left(\psi^*_{l,\text{plus}}\psi'_{l,\text{plus}} - \psi'^*_{l,\text{plus}}\psi_{l,\text{plus}}\right)$$

to the left of the singular point and the expression

$$i\kappa|a_{r,\text{plus}}|^2\left(-\psi^*_{r,\text{plus}}\psi'_{r,\text{plus}} + \psi'^*_{r,\text{plus}}\psi_{r,\text{plus}}\right)$$

to the right of the singular point. The first expression also took into account that $\psi_{l,\text{minus}} = \psi^*_{l,\text{plus}}$ and $\psi'_{l,\text{plus}} = \psi'^*_{l,\text{plus}}$, which directly follow from their explicit expressions. Combinations of wave functions in parentheses differ from zero and, in the general case, are equal with the opposite sign. Therefore, the equality of probabilistic currents implies

$$|a_{l,\text{plus}}|^2 - |a_{l,\text{minus}}|^2 = |a_{r,\text{plus}}|^2. \tag{17}$$

The resulting equations (16) and (17) are compatible only when $a_{l,\text{plus}} = -a_{l,\text{minus}}$. Then equation (16) states that $a_{r,\text{plus}} = 0$ that is, the intermediate singular potential is completely impenetrable.

6. TUNNELING OF INVERSE SQUARE AND STRONGLY SINGULAR POTENTIALS

Equation of state (1) for the inverse square potential has an exact analytical solution:

$$\psi_{r,1}(z) = \sqrt{z} J_\nu\left(\sqrt{\varepsilon} z\right), \quad \psi_{r,2}(z) = \sqrt{z} Y_\nu\left(\sqrt{\varepsilon} z\right) \tag{18}$$

for $z > 0$ and similarly for $z < 0$. Here, $J_\nu(\cdot)$ and $Y_\nu(\cdot)$ are the Bessel functions of the first and second kind, respectively, $\nu = \sqrt{0.25 + u_0}$.

A systematic analysis of solutions shows that for this form of the potential function, the solution to the tunneling problem depends on the sign u_0, that is, on whether the potential is a barrier or a well. In the case when $u_0 > 0$ the first solution in (18) vanishes at the singular point $z = 0$, and the second solution tends to infinity, the direct application of the continuity condition for the wave function becomes problematic. Here we approach it as a postulate of quantum mechanics, concretizing its meaning in the fact that with an asymptotic approach to the singular point on the left and right, the corresponding wave functions would diverge equally. We call this the quasi-continuity condition. In this context, it is important that the quasi-continuity completely preserves the singular content of the wave function and becomes the usual continuity condition if the problem is regularized. After some mathematics, the conditions for quasi-continuity and asymptotic absence of the reflected wave on the right-hand side of the potential lead, respectively, to

$$a_{l,2} = a_{r,2} \quad \text{and} \quad a_{r,1} = -ia_{r,2}. \tag{19}$$

And finally, combining (19) with the condition of continuity of the probabilistic current gives the generalized statement that

$$\mathrm{Im}[a_{l,1}] = a_{r,2}, \tag{20}$$

and $\mathrm{Re}[a_{l,1}]$ remains arbitrary. Then a free assumption about the real nature of the coefficient $a_{l,1}$ directly leads to $a_{r,1} = a_{r,2} = 0$, that is, the absence of a wave of matter to the right of the singularity point and, accordingly, to the expected result: complete impenetrability of the inverse square singular barrier.

In the case of a negative value u_0, both solutions (18) are equal to zero at the singular point $z = 0$. This ultimately makes it impossible to come to a definite answer about the possibility of tunneling the inverse square potential well within the framework of the approach presented in this article.

The strongly singular potential $\alpha > 2$ does not have an exact analytical solution for the Schrödinger equation (1), and we proceed from the approach developed in items 3 and 5. The answer essentially repeats the conclusions for the inverse square potential: the strongly singular potential barrier is completely impenetrable, and the potential well is beyond the capabilities of this approach.

7. CONCLUSION

In the problem of quantum tunneling of a singular potential, the regularization method is usually used, when the singularity is first removed in a narrow region around the singular point, the problem is solved for this prototype, and then the limiting transition of the narrowing of the regularization region to zero is made in the transmission and reflection coefficients. Another approach implies physically perceived conditions (the Friedrichs extension in the Hilbert space) for matching the wave function and its derivative on both sides of the singularity point. In particular, the one-dimensional Coulomb potential turns out to be impenetrable in both approaches. The preservation of the mathematical essence of the singularity, carried out in this article, dramatically changes the picture of tunneling at soft-singular and 1D Coulomb potentials. For example, in the case of a moderate singularity, the transparency of the potential remains finite even at the zero-energy boundary. In the other, the Coulomb case, the transparency of the potential at the same energy boundary fluctuates infinitely often between unity and zero, and when going to high energies it gradually decreases to zero.

Finally, potentials with a higher degree of singularity $\alpha > 1$, as in the regularization methods, exhibit complete impenetrability (while the case of a potential well $\alpha \geq 2$ remains outside the framework of the developed approach).

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