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TUNNELLING THROUGH A SINGULAR POTENTIAL BARRIER.

The Main Results

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1. Introduction

The quantum tunnelling is a phenomenon with a vast range of occurence in diverse branches of physics. One of the particularly interesting cases concerns the problem of conservation of topological charges in various field-theoretical models. It is believed on the basis of heuristic arguments /1/ that the transitions between states of different topological charges are tunnellings through an infinitely high energy barrier ; rigorous proofs of this assertion were given /2/ for the 2+1 dimensional O(3) σ-model, 2+1 dimensional electrodynamics and 3+1 dimensional Yang-Mills-Higgs theory. Such a tunnelling is forbidden semiclassically since the Euclidean action along any path crossing the barrier is infinite. The question naturally arises, whether the transitions are forbidden exactly too.

Motivated by this problem, we address ourselves in this paper with a considerably simpler question : we are going to study tunnelling through an infinitely high potential barrier V in one-dimensional quantum mechanics, particularly in the situations when the transition is semiclassically forbidden. There is no tunnelling, of course, when the infinitely high potential wall has a non-zero thickness. On the other hand, the answer is not a priori clear if $V(x)$ is finite almost everywhere with exception of one or more point singularities. For simplicity, we restrict our attention to the potentials that have just one point singularity placed at $x = 0$. The main result of the paper are two conditions, namely

$$\int_{-c}^{c} V(x)\, dx = \infty \qquad (1.1)$$

and

$$\int_{-c}^{c} x^2 V(x)^2\, dx = \infty \qquad (1.2)$$

for some $c>0$, which are sufficient for absence of the tunnelling provided the dynamics is determined by the potential V alone, or more explicitly, provided the formal Hamiltonian

$$H_1 = -\frac{d^2}{dx^2} + V(x) \qquad (1.3)$$

is essentially self-adjoint on its natural domain (a more detailed specification will be given in Section 2 below).

In the opposite case, one must choose a suitable self-adjoint extension of H_1 which is to play role of the Hamiltonian. Needless to say, this choice should be based on additional physical considerations ; roughly speaking, one must specify what happens when the particle reaches the centre of repulsion. A particular interest concerns the case when H_F , the extension in the sense of quadratic forms, is chosen for the Hamiltonian. In that case, the tunnelling is forbidden under the condition (1.1). It should be noted, that both the conditions (1.1) and (1.2) are fulfilled if V is a semiclassically impenetrable barrier, i.e.,

$$\int_{\mathbb{R}} (V(x)-E)_+^{1/2}\, dx = \infty \quad , \quad E>0 \ . \qquad (1.4)$$

For other self-adjoint extensions, however, conditions of this type might not ensure absence of the tunnelling. In order to illustrate this fact, we shall discuss in the second part of this paper the example of the barrier

$$V(x) = gx^{-2} \quad , \quad g>0 \ . \qquad (1.5)$$

If $g<\frac{3}{4}$, the corresponding operator H_1 is not essentially self-adjoint and has a family of self-adjoint extensions parametrized by 2×2 unitary matrices ; they can be constructed easily by the standard von Neumann method /3,4/. We shall evaluate there the transmission coefficient for each of the extensions ; it appears that the tunnelling is forbidden iff the corresponding matrix is diagonal.

There are many papers in which the motion in the field of a singular potential is treated (on various levels of mathematical rigour) ; see, e.g., Refs.5-10 and further references given therein. Most of them, however, concerns potentials in $\mathbb{R}^3$ with a singularity at the origin. The one-dimensional tunnelling discussed here has not been, up to our knowledge, considered earlier, though there are naturally some similarities to other works, especially in the example treated in the second part of the paper. It should be stressed also, that

the assumption about just one singularity in the potential V is not vital for our main results. The methods used to prove absence of the tunnelling under the conditions (1.1),(1.2) employ substantially the local behaviour of $V(.)$ only around the singularity, and therefore they are expected to work for the potentials V having a (finite or infinite) set of point singularities with no accumulation points.

2. Formulation of the problem

As mentioned above, we shall concentrate on the case of a non-negative barrier with one point singularity. Hence we adopt the following assumptions :

(a) V is Lebesgue measurable and $V(x)\geq 0$ holds a.e. in $\mathbb{R}$,

(b) $V(.)$ is bounded a.e. in $\mathbb{R}\setminus[-\eta,\eta]$ for each $\eta>0$.

Hamiltonian of the problem is, of course, a suitable self-adjoint extension of the symmetric operator

$$H_1 = H_0 + V \qquad (2.1)$$

with the domain $D(H_1)=D(H_0)\cap D(V)$, where $H_0\psi = -\psi''$ with $D(H_0) = AC^2[\mathbb{R}]$ (cf.Ref.3, Section X.1) and $(V\psi)(x)=V(x)\psi(x)$. Recall that $AC[M]$ denotes the set of all functions $f\in L^2(M)$ that are absolutely continuous in (each compact subinterval of) M with $f'\in L^2(M)$, and $AC^2[M]=\{f\in AC[M] : f'\in AC[M]\}$. We are particularly interested in the self-adjoint extension associated with the quadratic form

$$h : \ h(\psi) = \|\psi'\|^2 + \|V^{1/2}\psi\|^2 \qquad (2.2)$$

defined on $Q(h)=AC[\mathbb{R}]\cap D(V^{1/2})$. Since V is almost locally integrable and non-negative, the form h is closed and semibounded (Ref.12, Theorems 14.1.1 - 3). Consequently, there is a unique self-adjoint operator H_F associated with h , the Friedrichs extension of H_1 .

In spite of the eventual singularity at $x=0$, the scattering problem for H_F is well-posed if only V decays rapidly enough at infinity (for a general information about the rigorous scattering theory see Ref.3, Chapter XI, or Ref.11). To be specific, we assume that

(c) there are positive K , b , δ such that $V(x)\leq K|x|^{-1-\delta}$ for almost all $|x|>b$.

In such a case, the hypotheses of Theorem 14.2.1 in Ref.12 are easily seen to be fulfilled, so the following assertion is valid :

Proposition 2.1 : Under the assumptions (a)-(c), the wave operators $W_{\pm}(H_F, H_0)$ exist and are complete.

Next one has to make an assumption concerning the singularity of V. Semiclassical impenetrability of the barrier demands

$$\int_{\mathbb{R}} [V(x) - E]_+^p \, dx = \infty \tag{2.3}$$

with $p = \frac{1}{2}$ for a given energy E of the particle. For a greater generality, we shall consider this condition with other values of p too. Alternately, one may require

$$\int_{-c}^{c} V(x)^p \, dx = \infty \tag{2.4}$$

for some $c > 0$, as the following assertion shows :

Proposition 2.2 : Assume (a)-(c) and fix $p \in (0,1]$. Then the following conditions are equivalent :

(i) (2.3) holds for some $E > 0$,
(ii) (2.3) holds for all $E > 0$,
(iii) (2.4) holds for some $c > 0$,
(iv) (2.4) holds for all $c > 0$.

Proof : (i) $\Rightarrow$ (ii). The lhs of (2.3) is non-increasing with respect to E. Suppose it is finite for some $E_0 > 0$. We pick a positive $E \le \min\{E_0, K b^{-1-\delta}\}$ and denote $J_b = [-b, b]$, then

$$\int_{\mathbb{R}} [V(x) - E]_+^p \, dx \le \int_{\mathbb{R}\setminus J_b} [K|x|^{-1-\delta} - E]_+^p \, dx + \int_{J_b} [V(x) - E]_+^p \, dx \le$$

$$\le 2 \int_b^{(K/E)^{1/(1+\delta)}} [K y^{-1-\delta} - E]^p \, dx + 2b(E_0 - E)^p + \int_{\mathbb{R}} [V(x) - E_0]_+^p \, dx ,$$

because $[f(x)+g(x)]_+^p \le f_+(x)^p + g_+(x)^p$ holds for arbitrary functions f, g and $p \le 1$, and the last integral is certainly not lessened when J_b is replaced by $\mathbb{R}$. However, the first two terms on the rhs are finite so we arrived at a contradiction with (i).
(ii) $\Rightarrow$ (iii). To a given c, we can choose E such that $V(x) < E$ holds for almost all $|x| > c$. Then the lhs of (2.4) is bounded below by the lhs of (2.3) which is ∞ due to the assumption.
(iii) $\Rightarrow$ (iv). In view of (b), the integral of V^p is finite over each compact interval that does not contain zero.
(iv) $\Rightarrow$ (i). Now we pick c to a given E so that $V(x) < E$ holds

for almost all $|x| > c$. We denote as $J_c^{\pm}$ the sets $J_c \cap V^{(-1)}([E,\infty))$ and $J_c \cap V^{(-1)}([0,E))$, respectively. Then

$$\int_{\mathbb{R}} [V(x) - E]_+^p \, dx = \int_{J_c^+} [V(x) - E]^p \, dx \ge \int_{J_c^+} [V(x)^p - E^p] \, dx \ge$$

$$\ge \int_{J_c} V(x)^p \, dx - \int_{J_c^-} V(x)^p \, dx - 2cE^p \ge \int_{-c}^{c} V(x)^p \, dx - 4cE^p = \infty .$$ ■

Thus the assumption may be formulated as follows :

(d_p) for a given $p \in (0,1]$, any of the conditions (i)-(iv) holds.

Besides (d_p), we are going to consider one more condition of this type, namely

(e) the integral $\int_{-c}^{c} x^2 V(x)^2 \, dx$ is divergent for some (hence also for any) positive c.

Proposition 2.3 : (d_p) implies (d_q) if $0 < p \le q \le 1$. If $p < \frac{2}{3}$, then (d_p) implies (e). On the other hand, the conditions (d_p) and (e) are independent for $\frac{2}{3} < p \le 1$.

Proof : To a positive c, we denote $J_c^- = J_c \cap V^{(-1)}([0,1])$. Then

$$\int_{-c}^{c} V(x)^q \, dx \ge \int_{-c}^{c} V(x)^p \, dx + \int_{J_c^-} [V(x)^q - V(x)^p] \, dx \ge \int_{-c}^{c} V(x)^p \, dx - 2c$$

so the lhs is infinite if (d_p) holds. Next we use the Hölder inequality:

$$\int_{-c}^{c} V(x)^p \, dx \le \left(\int_{-c}^{c} |x|^{-2p/(2-p)} \, dx \right)^{(2-p)/2} \left(\int_{-c}^{c} x^2 V(x)^2 \, dx \right)^{p/2} .$$

If $p < \frac{2}{3}$, the first integral on the rhs is finite so the second assertion follows. Finally, one can consider the following examples. For a power-like potential, $V(x) = |x|^{-\alpha}$ with $p^{-1} \le \alpha < \frac{3}{2}$, the condition ($d_p$) is fulfilled, while (e) is not. On the other hand, the potential

$$V(x) = \begin{cases} n^3 & \dots \quad x \in \left(\frac{1}{n}, \frac{1}{n} + \frac{1}{n^5}\right), \quad n = 1,2,3,\dots \\ 0 & \dots \quad \text{otherwise} \end{cases}$$

gives $\int V(x)^p \, dx = \sum_n n^{3p-5}$ and $\int x^2 V(x)^2 \, dx = \sum_n (n^{-1} + O(n^{-5}))$, so (e) is valid, while (d_p) is fulfilled for no $p \in (0,1]$. ■

3. The main results

Our goal is to show that under the stated singularity conditions, a state localized initially on one of the halflines $\mathbb{R}_\pm$ stays confined there if its evolution is governed by the operator H_F associated with (2.2). Specifically, we are going to prove

Theorem 3.1 : Assume (a)-(c) and (d_1), then H_F commutes with the projections $E_\pm$ on $L^2(\mathbb{R}_\pm)$.

In view of Proposition 2.3, it gives the following result :

Corollary 3.2 : Let H_F be Hamiltonian of the problem. If the conditions (a)-(c) and (d_p) for some $p \in (0,1]$ are valid, then $\exp(-iH_F t)$ is reduced by $E_\pm$ for all $t \in \mathbb{R}$, so there is no tunnelling. In particular, it is true for $p = \frac{1}{2}$ in which case the tunnelling is semiclassically forbidden.

Proof of Theorem 3.1 : We denote $Q_1 = \{\psi \in AC[\mathbb{R}] : \psi(0) = 0\}$. For a vector $\psi \in Q(h)$, the function $V^{1/2}\psi$ must be square-integrable ; in view of (b), it is sufficient to investigate its behaviour in some neighbourhood of the origin only. Suppose $\psi(0) \neq 0$. Since ψ is (absolutely) continuous, there is a positive c such that $|\psi(x)| \geq \frac{1}{2}|\psi(0)|$ for $|x| < c$. Then

$$\int_{-c}^{c} V(x)\,|\psi(x)|^2\,dx \geq \frac{1}{4}\,|\psi(0)|^2 \int_{-c}^{c} V(x)\,dx$$

so we have a contradiction with (d_1). Consequently, $Q(h) \subset Q_1$.

Next we shall use this fact to prove the required commutativity. We define the restricted forms $h_\pm : h_\pm(\psi) = \|\psi'\|_\pm^2 + \|V^{1/2}\psi\|_\pm^2$, where $\|\psi\|_\pm := \int_{\mathbb{R}_\pm} |\psi(x)|^2\,dx$, with the domains $Q(h_\pm) = \{\psi \in L^2(\mathbb{R}_\pm) : \psi', V^{1/2}\psi \in L^2(\mathbb{R}_\pm)\ ,\ \lim_{x\to 0\pm} \psi(x) = 0\}$; they are obviously non-negative. Let us check that h_+ is closed. We take an arbitrary sequence $\{\psi_n\} \subset Q(h_+)$ such that $h_+(\psi_n - \psi_m) + \|\psi_n - \psi_m\|_+^2 \to 0$ as $n,m \to \infty$. By $\tilde\psi_n$, we denote the extension of ψ_n to $\mathbb{R}$ such that $\tilde\psi_n(x) = 0$ for $x < 0$. It is easy to see that $\tilde\psi_n$ is continuous and belongs to $Q(h)$ for $\psi_n \in Q(h_+)$, and $h(\tilde\psi_n) = h_+(\psi_n)$. Furthermore, $\|\tilde\psi_n\| = \|\psi_n\|_+$, so $h(\tilde\psi_n - \tilde\psi_m) + \|\tilde\psi_n - \tilde\psi_m\|^2 \to 0$ as $n,m \to \infty$. Since the form h is closed, there is $\tilde\psi \in Q(h)$ which is the limit of this Cauchy sequence, $h(\tilde\psi - \tilde\psi_n) + \|\tilde\psi - \tilde\psi_n\|^2 \to 0$ as $n \to \infty$. The function $\tilde\psi$ is continuous and $\tilde\psi(0) = 0$ so $\psi := \tilde\psi \restriction \mathbb{R}_+$ fulfils $\lim_{x\to 0+} \psi(x) = 0$. Obviously, $\psi \in Q(h_+)$

is the sought limit of the sequence $\{\psi_n\}$. Thus the form h_+ is closed, and by an analogous argument, h_- is closed.

Then there are unique self-adjoint operators $H_\pm$ on $L^2(\mathbb{R}_\pm)$ associated with the forms $h_\pm$. We construct the operator $\tilde H$ on $L^2(\mathbb{R}) = L^2(\mathbb{R}_-) \oplus L^2(\mathbb{R}_+)$ as the orthogonal sum, $H = H_- \oplus H_+$. This operator is self-adjoint and reduced by the projections $E_\pm$ by its definition. Furthermore, we define the quadratic form $\tilde h$ as $\tilde h = h_- \oplus h_+$, i.e., $\tilde h(\varphi_- \oplus \varphi_+) = h_-(\varphi_-) + h_+(\varphi_+)$ with $Q(\tilde h) = \{\varphi = \varphi_- \oplus \varphi_+ : \varphi_\pm \in Q(h_\pm)\}$. According to the definition, $\tilde h$ is non-negative and closed, and $\tilde H$ is the self-adjoint operator associated with it.

Finally, we shall compare the forms h and $\tilde h$. Let first $\varphi \in Q(h)$; we can write $\varphi = \tilde\varphi_- + \tilde\varphi_+$, where $\tilde\varphi_\pm = E_\pm\varphi$, or $\varphi = \varphi_- \oplus \varphi_+$ with $\varphi_\pm = \tilde\varphi_\pm \restriction \mathbb{R}_\pm$. In the same way as above, one may use $Q(h) \subset Q_1$ to check that $\varphi_\pm \in Q(h_\pm)$, i.e., $\varphi \in Q(\tilde h)$. On the other hand, consider a vector $\varphi = \varphi_- \oplus \varphi_+ \in Q(\tilde h)$. Extending the functions $\varphi_\pm$, we can write $\varphi = \tilde\varphi_- + \tilde\varphi_+$. The two functions are absolutely continuous and $\lim_{x\to 0\pm} \tilde\varphi_\pm(x) = 0$ so φ is absolutely continuous in (any finite subinterval of) $\mathbb{R}$. Further $\varphi_\pm' \in L^2(\mathbb{R}_\pm)$ implies $\varphi' \in L^2(\mathbb{R})$ and $V^{1/2}\varphi_\pm \in L^2(\mathbb{R}_\pm)$ implies $V^{1/2}\varphi \in L^2(\mathbb{R})$, so $\varphi \in Q(h)$ holds, too. Thus we have $Q(\tilde h) = Q(h)$ and the forms coincide,

$$h(\varphi) = \|\varphi'\|_-^2 + \|\varphi'\|_+^2 + \|V^{1/2}\varphi\|_-^2 + \|V^{1/2}\varphi\|_+^2 = h_-(\varphi_-) + h_+(\varphi_+) = \tilde h(\varphi)$$

for $\varphi \in Q(h)$. However, the self-adjoint operator associated with h is unique, and therefore $H_F = \tilde H$. ■

Using an operator argument, the following weaker assertion can be proved :

Theorem 3.3 : Under (a)-(c) and (e), the operator $\bar H_1$ commutes with $E_\pm$. Then there is no tunnelling if H_1 is essentially self-adjoint.

Proof : We denote $D_1 = \{\psi \in AC^2[\mathbb{R}] : \psi(0) = \psi'(0) = 0\}$. In order to determine $D(H_1)$, one must specify the behaviour of $V\psi$ around $x=0$. For $\psi \in AC^2[\mathbb{R}]$, one may use the first-order Taylor expansion with integral remainder, $\psi(x) = \psi(0) + \psi'(0)x + r_2(x)$, where

$$r_2(x) = x^2 \int_0^1 (1-t)\,\psi''(tx)\,dt \quad . \qquad (3.1a)$$

Estimating the integral by Schwartz inequality, we get

$$|r_2(x)| \leqslant 3^{-1/2} \left| \int_0^x |\psi''(y)|^2 dy \right|^{1/2} |x|^{3/2} \quad . \tag{3.1b}$$

In analogy with the preceding proof, (e) implies $\psi(0)=0$. Suppose $\psi'(0) \neq 0$. In that case, (3.1b) gives $|\psi(x)| \geqslant \frac{1}{2}|\psi'(0)x|$ for all sufficiently small x , and therefore

$$\int_{-c}^{c} V(x)^2 |\psi(x)|^2 dx \geqslant \frac{1}{4}|\psi'(0)|^2 \int_{-c}^{c} x^2 V(x)^2 dx$$

for some $c>0$. Consequently, $\psi'(0)=0$ holds too and $D(H_1) \subset D_1$.

Now the commutativity of $E_\pm$ with H_1 verifies easily. Since a vector $\psi \in D(H_1)$ can be represented by a continuously differentiable function that fulfils $\psi(0)=\psi'(0)=0$, we have $E_\pm\psi \in D(H_0)$. At the same time, $V\psi \in L^2(\mathbb{R})$ implies $VE_\pm\psi \in L^2(\mathbb{R})$, so $E_\pm\psi \in D(H_1)$. Check of the equality $H_1E_\pm\psi = E_\pm H_1\psi$ for such ψ is straightforward ; thus $E_\pm H_1 \subset H_1 E_\pm$. Finally, it is not difficult to see that if H_1 commutes with a bounded operator, the same is true for its closure $\overline{H}_1$. ∎

Let us collect now some simple properties of the operator H_1 and its extensions. We denote $H_{min} = H_1 \upharpoonright C_0^\infty(\mathbb{R} \setminus \{0\})$. An argument analogous to that presented in Ref.3, Appendix to Section X.1, shows that

$$D(H^*_{min}) \subset D^* \ , \tag{3.2a}$$

where $D^* = \{\psi \in L^2(\mathbb{R}) : \psi, \psi'$ absolutely continuous in $\mathbb{R} \setminus \{0\}$, $\psi'' \in L^2_{loc}(\mathbb{R} \setminus \{0\})$, $-\psi''+V\psi \in L^2(\mathbb{R}) \}$, and

$$H^*_{min} = -\psi'' + V\psi \quad . \tag{3.2b}$$

We have the following chain of inclusions,

$$H^*_{min} \supset H_1^* \supset H_F \supset \overline{H}_1 \supset H_1 \supset H_{min} \quad ; \tag{3.3}$$

if H_1 is not e.s.a., then other self-adjoint extensions may stand in the place of H_F .

These relations are important because they allow to find the deficiency subspaces of the operator H_1 by solving the ordinary differential equation

$$-\psi''(x) + V(x)\psi(x) = \pm i\psi(x) \quad ; \tag{3.4}$$

in particular, to verify the essential self-adjointness of H_1 in the case that the last equation has no solution within D^* . In the second part of the present paper, we shall treat in this way the potential barrier (1.5). The corresponding operator H_1 appears to be e.s.a. iff $g \geqslant \frac{3}{4}$, otherwise its deficiency indices are (2,2) . Since the equation (3.4) can be solved explicitly in this case, we shall be able to construct all self-adjoint extensions, and also to calculate the transmission coefficient to each of them.

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Диттрих Я., Экснер П. E2-84-352
Туннелирование сквозь сингулярный потенциальный барьер.
Главные результаты

Рассматривается квантовое туннелирование нерелятивистской частицы на прямой сквозь сингулярный потенциальный барьер V. В случае, когда гамильтониан $H_1 = -d^2/dx^2 + V(x)$ является, по существу, самосопряженным на своей естественной области определения, туннелирование запрещено для класса потенциалов, включающего полуклассически непроницаемые барьеры. Если H_1 не самосопряжен, по существу, тогда туннелирование, в общем, допустимо и зависит от самосопряженного расширения, выбранного в качестве гамильтониана данной проблемы. Среди них расширение по Фридрихсу дает запрет туннелирования для другого класса потенциалов, который опять включает полуклассически непроницаемые. Во второй части работы мы рассмотрим подробно пример $V(x) = gx^2$.

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Dittrich J., Exner P. E2-84-352
Tunnelling Through a Singular Potential Barrier.
The Main Results

Quantum tunnelling of a non-relativistic particle on the line through a singular potential barrier V is studied. If the Hamiltonian $H_1 = -d^2/dx^2 + V(x)$ is essentially self-adjoint on its natural domain, the tunnelling is forbidden for a class of potentials that includes the semiclassically impenetrable barriers. If H_1 is not essentially self-adjoint, occurence of the tunnelling is not excluded, in general, and depends on the self-adjoint extension we choose as Hamiltonian of the problem. Among them, the Friedrichs extension of H_1 yields no tunnelling for another class of potentials, which again includes the semiclassically impenetrable ones. In the second part of the paper, we shall treat in detail the example $V(x) = gx^2$.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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