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TUNNELLING THROUGH A SINGULAR POTENTIAL BARRIER. An Example: $V(x) = gx^{-2}$

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1. Introduction

We are going to continue the study of the quantum-mechanical tunnelling through a singular potential barrier started in the first part of this paper (Ref.1, hereafter referred to as [I]). We have considered there a non-relativistic particle on the line moving under influence of a potential V which was assumed to have a (repulsive) point singularity at $x=0$ (for a more detailed formulation of the problem - see Section 2 of [I]). We have obtained two conditions, namely

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

and

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

for some $c>0$, under which the tunnelling is forbidden provided the formal Hamiltonian $H_1 = H_0 + V$ is essentially self-adjoint (cf.Corollary 3.2 and Theorem 3.3 of [I]). Both these conditions are fulfilled particularly if the barrier is semiclassically impenetrable. Moreover, the tunneling is forbidden also in the case when H_1 is not e.s.a. and one chooses H_F, the Friedrichs extension of H_1, as the Hamiltonian of the problem.

2. The example of $V(x)=gx^{-2}$: construction of the self-adjoint extensions

Here we are going to illustrate that we may not generally replace the Friedrichs extension in the above assertion (i.e., in Corollary 3.2 of [I]) by another one. To this end, we shall treat in detail the particular barrier

$$V(x) = gx^{-2} \quad , \quad g>0 \quad . \tag{2.1}$$

This potential fulfils obviously the assumptions (a)-(c) from the Section 2 of [I], as well as (e) and (d_p) for $p \geq \frac{1}{2}$, thus all the respective conclusions apply.

Let us ask when $H_1 = H_0 + V$ is e.s.a. In view of the relations (3.2)-(3.4) of [I], the equation specifying the deficiency subspaces, $(H_1^* - i\lambda)\varphi = 0$ for $\lambda = \pm 1$, is simply related to the Bessel equation if we set

$$\nu = \left(g + \frac{1}{4}\right)^{1/2} \quad ; \tag{2.2}$$

its solutions on the halflines $\mathbb{R}_\pm$ are linear combinations of $(\pm x)^{1/2} H_\nu^{(k)}(e^{\pm\pi i \nu/4} x)$, $k = 1,2$. It is easy that none of them is square integrable if $\nu \geq 1$, i.e., if $g \geq \frac{3}{4}$, and therefore H_1 is e.s.a. in this case.

On the other hand, if $g \in (0, \frac{3}{4})$, or $\nu \in (\frac{1}{2}, 1)$, the deficiency subspaces $\mathcal{K}_\pm$ are two-dimensional and spanned by the vectors

$$\varphi_+^{(1)} : \varphi_+^{(1)}(x) = \theta(x)\, x^{1/2}\, H_\nu^{(1)}(\varepsilon x) \quad , \tag{2.3a}$$

$$\varphi_+^{(2)} : \varphi_+^{(2)}(x) = \varphi_+^{(1)}(-x) = -\theta(-x)\, (-x)^{1/2}\, \varepsilon^{-4\nu}\, H_\nu^{(2)}(\varepsilon x) \tag{2.3b}$$

and

$$\varphi_-^{(1)} : \varphi_-^{(1)}(x) = \overline{\varphi_+^{(1)}(x)} = \theta(x)\, x^{1/2}\, H_\nu^{(2)}(\bar{\varepsilon} x) \quad , \tag{2.3c}$$

$$\varphi_-^{(2)} : \varphi_-^{(2)}(x) = \overline{\varphi_+^{(2)}(x)} = -\theta(-x)\, (-x)^{1/2}\, \varepsilon^{4\nu}\, H_\nu^{(1)}(\bar{\varepsilon} x) \quad . \tag{2.3d}$$

Here and further on, we abbreviate $\varepsilon = e^{\pi i/4}$. The self-adjoint extensions of H_1 are then constructed in the standard way/2,3/. They are parametrized by the isometries $\mathcal{K}_+ \to \mathcal{K}_-$, i.e., by 2×2 matrices U whose elements fulfil the unitarity condition

$$\bar{u}_{1j} u_{1k} + \bar{u}_{2j} u_{2k} = \delta_{jk} \quad , \quad j,k = 1,2 \quad . \tag{2.4}$$

For a given U , we denote

$$\varphi_U^{(k)} = \varphi_+^{(k)} - u_{1k}\varphi_-^{(1)} - u_{2k}\varphi_-^{(2)} \quad , \quad k = 1,2 \quad . \tag{2.5}$$

According to the second von Neumann formula, the domain of the extension H_U of H_1 consists of the vectors $\psi = \varphi + (I-U)\varphi_+$,

where $\varphi_+ = c_1\varphi_+^{(1)} + c_2\varphi_+^{(2)}$, i.e.,

$$\psi = \varphi + c_1\varphi_U^{(1)} + c_2\varphi_U^{(2)} \tag{2.6a}$$

with $\varphi \in D(\overline{H}_1)$ and $c_1, c_2 \in \mathbb{C}$. The operator H_U acts on them as $H_U\psi = \overline{H}_1\varphi + i(I+U)\varphi_+$; in view of (3.2b) and the inclusions $H_U \subset H_1^* \subset \subset H^*_{min}$, one has

$$H_U\psi = -\psi'' + V\psi \quad . \tag{2.6b}$$

Let us look more closely how the functions of $D(H_U)$ behave around $x = 0$. We take $\psi \in D(H_U)$ and $\varphi \in D(H_U)$ with $\operatorname{supp}\varphi \subset [-n,n]$, then

$$(\varphi, H_U\psi) = \lim_{\eta\to 0+} \left(\int_{-n}^{-\eta} + \int_{\eta}^{n} \right) \bar{\varphi}(x)\, (-\psi''(x) + gx^{-2}\psi(x))\, dx \quad .$$

Since both ψ', φ' are absolutely continuous in any compact subinterval of $\mathbb{R}\setminus\{0\}$, one can integrate by parts obtaining in this way

$$(\varphi, H_U\psi) = (H_U\varphi, \psi) + \lim_{\eta\to 0+} \sum_{\alpha=\pm} \alpha\,(\bar{\varphi}(\alpha\eta)\psi'(\alpha\eta) - \bar{\varphi}'(\alpha\eta)\psi(\alpha\eta)) \quad .$$

Furthermore, to any $\varphi \in D(H_U)$ one can always find a sequence $\{\varphi_n\} \subset D(H_U)$ of functions supported by $[-n,n]$ such that $\varphi_n \to \varphi$, $H_U\varphi_n \to H_U\varphi$, e.g., by imposing (sufficiently smooth) cut-offs on φ . Then the last equality holds for arbitrary $\varphi, \psi \in D(H_U)$, and therefore the second term on its rhs must be zero for each such pair of vectors. This requirement can be reformulated as the following continuity condition

$$\lim_{x\to 0+} j(\varphi,\psi;x) = \lim_{x\to 0-} j(\varphi,\psi;x) \tag{2.7a}$$

for $\varphi, \psi \in D(H_U)$, where $j(\varphi,\psi;x) = \bar{\varphi}(x)\psi'(x) - \bar{\varphi}'(x)\psi(x)$. By a polarization-identity-type argument, it is further equivalent to

$$\lim_{x\to 0+} j_\psi(x) = \lim_{x\to 0-} j_\psi(x) \tag{2.7b}$$

for each $\psi \in D(H_U)$, where $j_\psi(x) = (2i)^{-1} j(\psi,\psi;x) = \operatorname{Im}\bar{\psi}(x)\psi'(x)$. Hence one can say that the domain of every particular extension H_U contains the vectors for which the probability current is continuous at $x = 0$.

A stronger assertion is valid for the vectors of $D(\overline{H}_1)$: one can take φ from the domain of $\overline{H}_1 = H_1^{**}$ and $\psi \in D(H_1^*)$, and repeat the above argument for $(\varphi, H_1^*\psi)$; it yields again the conditions (4.7a).

In the present case, however, one may always write $\psi=\psi_1+\psi_2$, where both ψ_1,ψ_2 belong to $D(H_1)$ and are supported by $(-\infty,0)$ and $(0,\infty)$, respectively. Consequently, one has

$$\lim_{x\to 0\pm} j(\varphi,\psi;x) = 0 \qquad (2.8)$$

for $\varphi\in D(\bar{H}_1)$ and $\psi\in D(H_1^*)$. Notice that the last relation is easily verified directly if $\varphi\in D(H_1)$ and $\psi\in\mathcal{K}_\pm$, because then $|\varphi(x)|\le K_\varphi|x|^{3/2}$ (cf.the proof of Theorem 3.3 in [I]) and the functions (2.3) behave near $x=0$ as follows

$$\varphi_+^{(1)}(x) = A\left[\bar{\varepsilon}^{\nu}x^{1/2-\nu} - B\bar{\varepsilon}^{3\nu}x^{1/2+\nu} + O(x^{5/2-\nu})\right] \ , \quad x>0 \ , \qquad (2.9a)$$

etc.(the remaining formulae are obtained by complex conjugation and/or replacement $x\to -x$), where

$$A = -\frac{i}{\pi}\,2^{\nu}\Gamma(\nu) = -\frac{2^{\nu}\,i}{\Gamma(1-\nu)\,\sin\nu\pi} \ , \quad B = 4^{-\nu}\,\frac{\Gamma(1-\nu)}{\Gamma(1+\nu)} \ . \qquad (2.9b)$$

On the other hand, (2.8) need not be true if neither φ nor ψ is contained in $D(\bar{H}_1)$. In view of (2.6a), we are particularly interested in the case when φ,ψ are of the form (2.5). The limits can be calculated with the help of (2.9) and (2.4) ; they equal

$$\lim_{x\to 0\pm} j(\varphi_U^{(1)},\varphi_U^{(1)};x) = \frac{2i}{\pi}\,|u_{21}|^2 \sec\frac{\nu\pi}{2} \ , \qquad (2.10a)$$

$$\lim_{x\to 0\pm} j(\varphi_U^{(2)},\varphi_U^{(2)};x) = -\frac{2i}{\pi}\,|u_{12}|^2 \sec\frac{\nu\pi}{2} \ , \qquad (2.10b)$$

$$\lim_{x\to 0\pm} j(\varphi_U^{(1)},\varphi_U^{(2)};x) = -\frac{2i}{\pi}\,\bar{u}_{11}u_{12} \sec\frac{\nu\pi}{2} \ . \qquad (2.10c)$$

We see that, in general, the probability current for $\psi\in D(H_U)$ need not vanish at $x=0$ unless U is diagonal. It indicates that the tunnelling might occur in such cases. In the next section, we shall confirm this conjecture by evaluating the transmission coefficient. Notice that the matrix $U=U_F$ referring to the Friedrichs extension is diagonal : we have shown in the proof of Theorem 3.1 of [I] that $D(H_F)\subset Q(h)\subset Q_1$, and threfore one has to require $\lim_{x\to 0\pm}\varphi_U^{(k)}(x)=0$. It yields easily

$$U_F = -\bar{\varepsilon}^{2\nu} I \ . \qquad (2.11)$$

<u>Remark 2.1</u> : In the above considerations, closedness of H_1 is not required. Before proceeding further, we would like to mention an

elegant proof of this property which, however, works for $g>\frac{3}{4}$ only. It is based on the canonical commutation relations. We write $H_1=(P^2+\frac{3}{4}Q^{-2})+(g-\frac{3}{4})Q^{-2}$ and apply it on a vector ψ of a suitable domain, say, $C_0^\infty(\mathbb{R}\setminus\{0\})$. It gives

$$\|H_1\psi\|^2 = \|(P^2+\tfrac{3}{4}Q^{-2})\psi\|^2 + (g^2-\tfrac{9}{16})\,\|Q^{-2}\psi\|^2 + (g-\tfrac{3}{4})\,(\psi,(P^2Q^{-2}+Q^{-2}P^2)\psi).$$

Using the relation $[P,Q^{-1}]\psi = iQ^{-2}\psi$, one can rewrite the last term as follows

$$(\psi,(P^2Q^{-2}+Q^{-2}P^2)\psi) = \tfrac{1}{2}\,\|(3PQ^{-1}-Q^{-1}P)\psi\|^2 - \tfrac{3}{2}\,\|Q^{-2}\psi\|^2 \ .$$

Omitting the non-negative terms, we get the inequality

$$\|H_1\psi\|^2 \ge (g-\tfrac{3}{4})^2\,\|Q^{-2}\psi\|^2 \ , \quad \psi\in C_0^\infty(\mathbb{R}\setminus\{0\}) \ . \qquad (2.12)$$

The remaining part of the argument is simple (cf.the analogous problem treated in Ref.4 , Proposition 1). Since $g>\frac{3}{4}$, H_{min} is e.s.a. and the relations (3.2) of [I] show that $C_0^\infty(\mathbb{R}\setminus\{0\})$ is a core for H_1 . To a vector $\psi\in D(\bar{H}_1)$, we take a sequence $\{\psi_n\}\subset C_0^\infty(\mathbb{R}\setminus\{0\})$, $\psi_n\to\psi$, then $\{H_1\psi_n\}$ is Cauchy and the same is true for $\{Q^{-2}\psi_n\}$ due to (2.12), and for $\{P^2\psi_n\}$ too since $P^2\psi_n = H_1\psi_n - gQ^{-2}\psi_n$. However, both P^2 and Q^{-2} are closed so $\psi\in D(P^2)\cap D(Q^{-2}) = D(H_1)$.

3. <u>The transmission coefficient</u>

Now we shall discuss scattering on the barrier (2.1) restricting ourselves to the non-trivial case, $0<g<\frac{3}{4}$, only. We use the time-independent setting, because it is simpler, and at the same time, it allows to illustrate the main point, namely that the dynamics is determined by the self-adjoint extension H_U chosen to play the role of Hamiltonian. Hence we are going to work with the functions which obey all the appropriate requirements <u>locally</u> but eventually do not exhibit the overall square integrability. In order to get the rigorous Hilbert-space (time-dependent) scattering theory, one should consider the motion of wavepackets composed of the plane-wave solutions constructed below ; but we are not going to pursue this task.

Given $E>0$, we are looking for solutions of the stationary Schrödinger equation

$$-\psi''(x) + gx^{-2}\psi(x) = E\psi(x) \qquad (3.1)$$

assuming they are of the form analogous to (2.6a),

$$\psi = \psi_1 + c_1\psi_U^{(1)} + c_2\psi_U^{(2)} \quad , \tag{3.2}$$

where ψ_1 belongs locally to $D(\bar{H}_1)$. The equation (3.1) can be then rewritten as

$$-\psi_1''(x) + (gx^{-2} - E)\psi_1(x) = \chi(x) \quad , \tag{3.3a}$$

where χ expresses through the functions (2.3) as

$$\chi(x) = \theta(x)\left[c_+^{(1)}\varphi_+^{(1)}(x) + c_-^{(1)}\varphi_-^{(1)}(x)\right] + \theta(-x)\left[c_+^{(2)}\varphi_+^{(2)}(x) + c_-^{(2)}\varphi_-^{(2)}(x)\right] \tag{3.3b}$$

with

$$c_+^{(k)} = c_k(E-i) \quad , \quad c_-^{(k)} = -(c_1u_{k1} + c_2u_{k2})(E+i) \quad , \quad k = 1,2 \quad . \tag{3.3c}$$

The function χ is C^∞ in $\mathbb{R}\setminus\{0\}$ so the same is true for ψ_1 . It can be seen as follows : $\psi_1'' = (gx^{-2}-E)\psi_1 - \chi \in C^1(\mathbb{R}\setminus\{0\})$, because ψ_1 belongs locally to $D(\bar{H}_1) \subset D^*$ (cf.(3.2a) of [I]), then one has to derivate successively the last relation.

First we shall solve the equation (3.3a) for $x > 0$. We start with the related homogeneous equation whose solution is easily found to be $\psi_0 = \alpha_1\psi_{01} + \alpha_2\psi_{02}$, where

$$\psi_{0k}(x) = x^{1/2}H^{(k)}(\lambda x) \quad , \quad k = 1,2 \quad , \tag{3.4a}$$

where $\lambda = E^{1/2}$. The Wronskian of these functions can be determined from their asymptotic behaviour, either for $x \to \infty$ or for $x \to 0+$,

$$\psi_{01}(x) = \overline{\psi_{02}(x)} = A\left[E^{-\nu/2}x^{1/2-\nu} - B\bar{\varepsilon}^{4\nu}E^{\nu/2}x^{1/2+\nu} + O(x^{5/2-\nu})\right]; \tag{3.5}$$

one has $W(\psi_{01},\psi_{02}) = 4/\pi i$. Next we suppose the general solution to (3.3a) to be of the form

$$\psi_1(x) = \alpha_1(x)\psi_{01}(x) + \alpha_2(x)\psi_{02}(x) \quad . \tag{3.4b}$$

The corresponding system of first-order equations for the functions α_k is easily solved giving

$$\psi_1(x) = \frac{\pi i}{4}\psi_{01}(x)\int_0^x \chi(y)\psi_{02}(y)\,dy - \frac{\pi i}{4}\psi_{02}(x)\int_0^x \chi(y)\psi_{01}(y)\,dy + \alpha_1\psi_{01}(x) + \alpha_2\psi_{02}(x) \quad , \tag{3.6}$$

where the constants α_1,α_2 are arbitrary up to now. In order to fix them, let us look at the behaviour of ψ_1 near the origin. It can be found from the formulae (2.9),(3.3) and (3.5). A short calculation shows that the leading-order terms (behaving as $x^{5/2-3\nu}$) in the first two expressions of (3.6) cancel mutually, and the asymptotics is determined by the last two expressions, specifically

$$\psi_1(x) = (\alpha_1 - \alpha_2)AE^{-\nu/2}|x|^{1/2-\nu} - AB(\alpha_1\bar{\varepsilon}^{4\nu} - \alpha_2\varepsilon^{4\nu})E^{\nu/2}|x|^{1/2+\nu} + O(|x|^{5/2-\nu}) \quad . \tag{3.7}$$

Before proceeding further, let us look for the solution to (3.3a) for $x < 0$. It can be found easily : $\psi_1(x) = \tilde{\psi}_1(-x)$, where $\tilde{\psi}_1$ fulfils the same equation as ψ_1 with replacement of $\chi(x)$ by $\chi(-x)$. Since $\varphi_\pm^{(2)}(x) = \varphi_\pm^{(1)}(-x)$, the function $\tilde{\psi}_1$ differs from ψ_1 just by the coefficients : in the first two terms of (3.6) $c_\pm^{(2)}$ stand in the place of $c_\pm^{(1)}$, and α_1,α_2 may assume other values. With this difference, the asymptotics of ψ_1 for $x \to 0-$ is again given by (3.7).

Lemma 3.1 : Let a function $\psi \in L^2_{loc}(\mathbb{R})$ fulfil the following conditions:
(a) ψ,ψ' are absolutely continuous in $\mathbb{R}\setminus\{0\}$,
(b) there is a positive η such that $\psi'' \in L^2_{loc}(\mathbb{R}\setminus[-\eta,\eta])$,
(c) it holds $\psi(x) = [a_1x^{1/2-\nu} + a_2x^{1/2+\nu}]\theta(x) + [a_3(-x)^{1/2-\nu} + a_4(-x)^{1/2+\nu}]\theta(-x) + f(x)$, where f belongs locally to $D(H_1)$ (equivalently : f' is absolutely continuous in $\mathbb{R}$ and the functions f'' , $x^{-2}f$ belong to $L^2(-\eta,\eta)$).
Then either $a_1 = \cdots = a_4 = 0$ or ψ does not belong locally to $D(\bar{H}_1)$.

Proof : We write the function $\sigma \equiv \psi - f$ as $\varphi - \omega$, where φ is a suitable linear combination of the functions (2.3) and ω is regular at the origin. Using (2.9) and the fact that $\sin(\nu\pi/2)$ is non-zero for $\nu \in (\frac{1}{2},1)$, we see that φ is determined uniquely by the numbers a_j and that $\omega(x) = O(|x|^{5/2-\nu})$ near the origin. Then ω belongs locally to $D(H_1) \subset D(\bar{H}_1)$ and the same is true for $f - \omega = \psi - \varphi$ in view of the assumption (c). Suppose that ψ belongs locally to $D(\bar{H}_1)$, then the same should hold true for φ . Moreover, φ is square-integrable so $\varphi \in D(\bar{H}_1)$. However, φ lies in the subspace $\mathcal{K}_+ \oplus_{H_1} \mathcal{K}_-$

of $D(H_1^*)$ that is H_1-orthogonal to $D(\overline{H}_1)$ (Ref.4, Section X.1). It is possible only if $\varphi = 0$, or equivalently, $a_1 = \cdots = a_4 = 0$. ∎

The function ψ_1 is supposed to be locally of $D(\overline{H}_1)$ so the above lemma implies easily that the last two terms on the rhs of (3.6) must vanish, and similarly for $\tilde{\psi}_1$. Now we express the obtained solution more explicitly substituting for χ from (3.3b). We denote

$$J_{k\pm}(x) = \int_x^\infty \varphi_\pm^{(1)}(y)\psi_{0k}(y)\,dy \quad , \quad x \geq 0 \quad , \tag{3.8a}$$

$$J_{k\pm} = J_{k\pm}(0) \quad . \tag{3.9}$$

The asymptotic behaviour of $J_{k\pm}(.)$ for $x \to \infty$ can be found using that of the cylindrical functions in (2.3),(3.4a) : there is a constant K (depending on E) such that

$$|J_{k\pm}(x)| \leq K \exp(-2^{-1/2}x) \quad , \quad x \geq 0 \quad . \tag{3.8b}$$

The function ψ_1 for $x > 0$ can be now rewritten as

$$\begin{aligned}\psi_1(x) = \frac{\pi i}{4}\left[c_+^{(1)}(J_{2+} - J_{2+}(x)) + c_-^{(1)}(J_{2-} - J_{2-}(x))\right]\psi_{01}(x) - \\ - \frac{\pi i}{4}\left[c_+^{(1)}(J_{1+} - J_{1+}(x)) + c_-^{(1)}(J_{1-} - J_{1-}(x))\right]\psi_{02}(x) \quad ,\end{aligned} \tag{3.10a}$$

and due to (3.4a),(3.8b) , its asymptotic behaviour for $x \to \infty$ is the following

$$\begin{aligned}\psi_1(x) = \frac{i}{2}\left(\frac{\pi}{2\lambda}\right)^{1/2}\Big\{(c_+^{(1)}J_{2+} + c_-^{(1)}J_{2-}) \exp\left[i(\lambda x - \frac{\nu\pi}{2} - \frac{\pi}{4})\right] - \\ - (c_+^{(1)}J_{1+} + c_-^{(1)}J_{1-}) \exp\left[-i(\lambda x - \frac{\nu\pi}{2} - \frac{\pi}{4})\right]\Big\} + O(x^{-1}) \quad ,\end{aligned} \tag{3.11a}$$

where again $\lambda = E^{1/2}$. Similarly, one has the expression

$$\begin{aligned}\psi_1(x) = \frac{\pi i}{4}\left[c_+^{(2)}(J_{2+} - J_{2+}(-x)) + c_-^{(2)}(J_{2-} - J_{2-}(-x))\right]\psi_{01}(-x) - \\ - \frac{\pi i}{4}\left[c_+^{(2)}(J_{1+} - J_{1+}(-x)) + c_-^{(2)}(J_{1-} - J_{1-}(-x))\right]\psi_{02}(-x)\end{aligned} \tag{3.10b}$$

for $x < 0$, which behaves for $x \to -\infty$ as

$$\begin{aligned}\psi_1(x) = \frac{i}{2}\left(\frac{\pi}{2\lambda}\right)^{1/2}\Big\{(c_+^{(2)}J_{2+} + c_-^{(2)}J_{2-}) \exp\left[-i(\lambda x + \frac{\nu\pi}{2} + \frac{\pi}{4})\right] - \\ - (c_+^{(2)}J_{1+} + c_-^{(2)}J_{1-}) \exp\left[i(\lambda x + \frac{\nu\pi}{2} + \frac{\pi}{4})\right]\Big\} + O(|x|^{-1}) \quad .\end{aligned} \tag{3.11b}$$

In order to make use of the relations (3.11), we should know the coefficients $J_{k\pm}$ explicitly. It can be easily achieved (cf.Ref.5, 6.521.3 and 8.407.1) ; one has

$$J_{1+} = \frac{2}{\pi}\,\frac{\varepsilon^{4\nu}}{\sin\nu\pi}\,\frac{\bar{\varepsilon}^{\nu}E^{\nu/2} - \varepsilon^{\nu}E^{-\nu/2}}{E-i} \quad , \tag{3.12a}$$

$$J_{1-} = \frac{2}{\pi}\,\frac{\varepsilon^{3\nu}E^{-\nu/2} - \bar{\varepsilon}^{3\nu}E^{\nu/2}}{\sin\nu\pi\,(E+i)} \quad , \tag{3.12b}$$

$$J_{2+} = \overline{J}_{1-} \quad , \quad J_{2-} = \overline{J}_{1+} \quad . \tag{3.12c}$$

Now the crucial point is that the functions $\varphi_U^{(k)}$ in (3.2) decay exponentially at infinity. Thus the asymptotic behaviour of ψ coincides with that of ψ_1, and it is fully determined by the choice of the coefficients $c_\pm^{(k)}$. One has to know the correspondences $(c_+^{(1)},c_-^{(1)}) \leftrightarrow (c_1,c_2) \leftrightarrow (c_+^{(2)},c_-^{(2)})$. Two cases should be distinguished :

(i) <u>the matrix U is diagonal</u>. Then the pairs $c_\pm^{(1)}$ and $c_\pm^{(2)}$ are independent : the relations (3.3c) give

$$c_-^{(k)} = -\,u_{kk}\,\frac{E+i}{E-i}\,c_+^{(k)} \quad , \quad k = 1,2 \quad . \tag{3.13}$$

Consider the situation when one of these pairs is zero, say, $c_\pm^{(2)} = 0$. Then the formulae (3.11a),(3.12c) and (3.13) yield the asymptotics

$$\begin{aligned}\psi(x) = \frac{i}{2}\left(\frac{\pi}{2\lambda}\right)^{1/2} c_+^{(1)}\Big\{(J_{2+} - u_{11}\frac{E+i}{E-i}J_{2-}) \exp\left[i(\lambda x - \frac{\nu\pi}{2} - \frac{\pi}{4})\right] + \\ + u_{11}\frac{E+i}{E-i}\,\overline{(J_{2+} - u_{11}\frac{E+i}{E-i}J_{2-})} \exp\left[-i(\lambda x - \frac{\nu\pi}{2} - \frac{\pi}{4})\right]\Big\} + O(x^{-1})\end{aligned} \tag{3.14a}$$

for $x \to \infty$. On the other hand $c_\pm^{(2)} = 0$ implies $c_2 = 0$ so the relations (3.2),(2.5) together with $u_{21} = 0$ give $\psi(x) = \psi_1(x)$ for $x < 0$. In that case, however,

$$\psi(x) = 0 \quad , \quad x < 0 \quad , \tag{3.14b}$$

holds due to (3.10b). Hence we have total reflection in this case ; the phase shift of the reflected wave can be easily derived from (3.14a).

(ii) <u>the matrix U is non-diagonal</u>. Now the appropriate determinants are non-zero so the correspondence $(c_+^{(1)},c_-^{(1)}) \leftrightarrow (c_+^{(2)},c_-^{(2)})$ is bijective. We choose the initial conditions in such a way that we have the transmitted wave on the positive semiaxis only, i.e.,

$$c_+^{(1)}J_{1+}+c_-^{(1)}J_{1-}=0 \quad . \qquad (3.15a)$$

Then the reflection and transmission coefficients are defined by the expressions

$$R = R_\nu(E;U) = \left|\frac{c_+^{(2)}J_{2+}+c_-^{(2)}J_{2-}}{c_+^{(2)}J_{1+}+c_-^{(2)}J_{1-}}\right|^2 \qquad (3.15b)$$

and

$$T = T_\nu(E;U) = \left|\frac{c_+^{(1)}J_{2+}+c_-^{(1)}J_{2-}}{c_+^{(2)}J_{1+}+c_-^{(2)}J_{1-}}\right|^2 \quad , \qquad (3.15c)$$

respectively. Using (3.12c) together with the unitarity condition (2.4), one can check that the equality $|c_+^{(2)}J_{2+}+c_-^{(2)}J_{2-}|^2 + |c_+^{(1)}J_{2+}+c_-^{(1)}J_{2-}|^2 = |c_+^{(2)}J_{1+}+c_-^{(2)}J_{1-}|^2$ holds if (3.15a) is valid, i.e.,

$$R + T = 1 \quad . \qquad (3.16)$$

Let us now express the transmission coefficient more explicitly. The system of equations for $c_\pm^{(2)}$ that follows from (3.3c) is easily solved. Further $c_+^{(1)}$ and $c_-^{(1)}$ are related by (3.15a), so we obtain

$$c_+^{(2)} = -\frac{1}{u_{12}}\,\frac{E-i}{E+i}\,(1+u_{11}\beta)\,c_-^{(1)} \quad ,$$

$$c_-^{(2)} = \left[-u_{21}\beta + \frac{u_{22}}{u_{12}}(1+u_{11}\beta)\right]c_-^{(1)} \quad ,$$

where

$$\beta = -\frac{E+i}{E-i}\,\frac{J_{1-}}{J_{1+}} = \varepsilon^{6\nu}\,\frac{1-\bar\varepsilon^{6\nu}E^\nu}{1-\bar\varepsilon^{2\nu}E^\nu} \quad . \qquad (3.17a)$$

Substituting now to (3.15c) and denoting

$$\gamma = \frac{J_{2+}}{J_{1+}} = -\,\frac{1-\varepsilon^{6\nu}E^\nu}{1-\bar\varepsilon^{2\nu}E^\nu} \quad , \qquad (3.17b)$$

we arrive after a short calculation at the expression

$$T = \left|\frac{\gamma(\beta-\bar\beta^{-1})u_{12}}{1+\beta\,\mathrm{Tr}\,U+\beta^2\det U}\right|^2 \quad . \qquad (3.17c)$$

After some more simple manipulations, we can rewrite it in the following final form

$$T_\nu(E;U) = 16\,|u_{12}|^2\sin^2\nu\pi\,\sin^2\frac{\nu\pi}{2}\,|aE^\nu+b+cE^{-\nu}|^{-2} \quad , \qquad (3.18a)$$

where

$$a = a_\nu(U) = \bar\varepsilon^{4\nu}\left[1+\varepsilon^{2\nu}\,\mathrm{Tr}\,U+\varepsilon^{4\nu}\det U\right] \quad , \qquad (3.18b)$$

$$b = b_\nu(U) = -2\,\bar\varepsilon^{2\nu}\left[1+\varepsilon^{4\nu}\cos\frac{\nu\pi}{2}\,\mathrm{Tr}\,U+\varepsilon^{8\nu}\det U\right] \quad , \qquad (3.18c)$$

$$c = c_\nu(U) = 1+\varepsilon^{6\nu}\,\mathrm{Tr}\,U+\varepsilon^{12\nu}\det U \quad . \qquad (3.18d)$$

Let us collect some simple properties of T :

Theorem 5.2 : Let $E>0$ and $\nu=(g+\frac{1}{4})^{1/2}\in(\frac{1}{2},1)$. The transmission coefficient $T_\nu(E;U)$ referring to the self-adjoint extension H_U of H_1 with the potential (2.1) is then given by the formulae (3.18), where the coefficients (3.18b-d) cannot be simultaneously zero. It assumes values from $[0,1]$ and depends continuously on ν,E,U . In particular, for a diagonal matrix U we have total reflection, $T_\nu(E;U)=0$. For a non-diagonal U , the following alternative is valid :

either U is unitarily equivalent to the matrix $-\bar\varepsilon^4\begin{pmatrix}\varepsilon^{2\nu} & 0\\ 0 & \bar\varepsilon^{2\nu}\end{pmatrix}$ and

$$T = 4\,|u_{12}|^2\cos^2\frac{\nu\pi}{2} \qquad (3.19)$$

is energy-independent,

or at most one of the coefficients (3.18b-d) can be zero. In that case, T has the following asymptotic behaviour

$$T_\nu(E;U) = 16\,|u_{12}|^2\sin^2\nu\pi\,\sin^2\frac{\nu\pi}{2}\,f(E) \quad , \qquad (3.20a)$$

where

$$f(E) = |c|^{-2}E^{2\nu}-2|c|^{-4}\mathrm{Re}\,\bar b c\,E^{3\nu}+O(E^{4\nu}) \quad , \quad c\neq 0 \quad , \qquad (3.20b)$$

$$f(E) = |b|^{-2}-2|b|^{-4}\mathrm{Re}\,\bar a b\,E^{\nu}+O(E^{2\nu}) \quad , \quad c=0 \quad , \qquad (3.20c)$$

holds for $E\to 0+$, and similarly

$$f(E) = |a|^{-2}E^{-2\nu}-2|a|^{-4}\mathrm{Re}\,\bar a b\,E^{-3\nu}+O(E^{-4\nu}) \quad , \quad a\neq 0 \quad , \qquad (3.20d)$$

$$f(E) = |b|^{-2}-2|b|^{-4}\mathrm{Re}\,\bar b c\,E^{-\nu}+O(E^{-2\nu}) \quad , \quad a=0 \quad , \qquad (3.20e)$$

for $E\to\infty$.

For fixed E and U , the transmission coefficient tends not necessarily to 0 as $g \to \frac{3}{4}-$ and to 1 as $g \to 0+$. In fact, we have

$$\lim_{\nu \to 1/2+} T_\nu(E;U) = 1 \tag{3.21a}$$

iff the matrix U is of the form $2^{-1/2}\begin{pmatrix} i & e^{-i\omega} \\ e^{i\omega} & i \end{pmatrix}$ with $\omega \in \mathbb{R}$; otherwise there are at most three values of E for which (3.21a) can hold. On the other hand,

$$\lim_{\nu \to 1-} T_\nu(E;U) = 0 \tag{3.22a}$$

holds almost everywhere : there are at most two values of E where the limit is non-zero for a non-diagonal U , namely

$$E = \frac{\cos\alpha}{1 - \sin\alpha} \quad , \tag{3.22b}$$

where $e^{i\alpha}$ is an eigenvalue of U such that $\alpha \in (-\frac{\pi}{2}, \frac{\pi}{2})$.

<u>Proof</u> : The inequality $0 < T < 1$ follows from (3.15),(3.16) . Each of the coefficients (3.18b-d) may be zero (examples of such matrices U can be easily found), but they cannot vanish simultaneously. Suppose, e.g., that $a = b = 0$. The relations (3.18b,c) then yield

$$\det U = -\bar{\varepsilon}^{4\nu} - \bar{\varepsilon}^{2\nu}\,\mathrm{Tr}\,U = -\bar{\varepsilon}^{8\nu} - \bar{\varepsilon}^{4\nu}\cos\frac{\nu\pi}{2}\,\mathrm{Tr}\,U \tag{3.23a}$$

and the last inequality further implies

$$\mathrm{Tr}\,U = -2\bar{\varepsilon}^{2\nu} \quad . \tag{3.23b}$$

The relations (3.23) are fulfilled iff $U = -\bar{\varepsilon}^{2\nu} I$, then $a = b = 0$, while $c = (1 - \varepsilon^{4\nu})^2$ is non-zero. Similarly, $b = c = 0$ is possible for $U = -\bar{\varepsilon}^{6\nu} I$ only, in which case $a = \bar{\varepsilon}^{4\nu}(1 - \bar{\varepsilon}^{4\nu})^2 \neq 0$. Both these U are multiples of the unit matrix so the transmission coefficient is zero for them. For a non-diagonal matrix U therefore, either $a = c = 0$ or at least two of the coefficients are non-zero. In the first case, the relations (3.18b,d) determine uniquely the values

$$\mathrm{Tr}\,U = -2\bar{\varepsilon}^{4\nu}\cos\frac{\nu\pi}{2} \quad , \quad \det U = \bar{\varepsilon}^{2\nu} \quad ,$$

which can be achieved just for the matrices U that are unitarily equivalent to the above written one. The relation (3.19) then follows readily from (3.18) and (3.23). Check of the relations (3.20) is elementary.

In order to prove continuity of $T_\nu(E;U)$, one has to verify that the denominator in (3.18a) does not vanish in the allowed region of parameters. In view of (3.17), it equals $(1 + \beta\,\mathrm{Tr}\,U + \beta^2 \det U)(1 - \bar{\varepsilon}^{2\nu}E^\nu)$ and since the last factor is non-zero, we must solve the corresponding quadratic equation for β . Its roots are easily seen to be $\beta_k = -\exp(-i\alpha_k)$, $k = 1,2$, where $\exp(i\alpha_k)$ are eigenvalues of U . Hence we have to solve the equation

$$\beta = \varepsilon^{6\nu}\,\frac{1 - \bar{\varepsilon}^{6\nu}E^\nu}{1 - \bar{\varepsilon}^{2\nu}E^\nu} = e^{i\alpha} \quad , \quad \alpha = \alpha_1, \alpha_2 \quad . \tag{3.24a}$$

Obviously $|\beta| = 1$, and it yields the condition $\sin\nu\pi \sin\frac{\nu\pi}{2} = 0$ which cannot be fulfilled for $\nu \in (\frac{1}{2}, 1)$.

Let us pass to the limits in ν . The equation (3.24a) has no solutions for $\nu = \frac{1}{2}$ as well, so we have

$$\lim_{\nu \to 1/2+} T_\nu(E;U) = 8|u_{12}|^2 \Big| (-i + \bar{\varepsilon}\,\mathrm{Tr}\,U + \det U)E^{1/2} + 2\varepsilon^3(1 + 2^{-1/2} i\,\mathrm{Tr}\,U - \det U) - i(i - \varepsilon\,\mathrm{Tr}\,U + \det U)E^{-1/2} \Big|^{-2} \tag{3.21b}$$

with the rhs properly defined. It yields particularly (3.21a) if $a = c = 0$ and $|u_{12}| = 2^{-1/2}$ what is possible just for the matrices written above. If these requirements are not fulfilled, then (3.21a) can hold only for the values of E where the denominator in the rhs of (3.21b) reaches its minimum. This condition leads to a fourth-order equation for $E^{-1/2}$. It has at most four real roots, among them one necessarily negative, if both a,c are non-zero, and at most one in the remaining cases.

On the other hand, the equation (3.24a) has two solutions E_k , $k = 1,2$, if $\nu = 1$; they are eventually equal to each other (if $\alpha_1 = \alpha_2$) or to ∞ (if $\alpha_k = \frac{\pi}{2}$). It is easy to find that they are given by (3.22b), where only the case $\alpha \in (-\frac{\pi}{2}, \frac{\pi}{2})$ is interesting giving a positive solution. With the exception of $E = E_k$, the relation (3.22a) holds. If E equals to $E_k > 0$, one obtains

$$\lim_{\nu \to 1-} T_\nu(E_k;U) = 16\pi^2 |u_{12}|^2\, |d(E_k;U)|^{-2} \quad , \tag{3.22c}$$

where

$$d(E;U) = -\frac{d}{d\nu}\left[a_\nu(U)E^\nu + b_\nu(U) + c_\nu(U)E^{-\nu} \right]_{\nu=1} \quad ; \tag{3.22}$$

the last expression cannot be zero at $E = E_k$ since T is bounded by 1 . ■

Hence we have confirmed the conjecture formulated in the preceding section : the tunnelling actually occurs for the barrier (2.1) with $g \in (0, \frac{3}{4})$, unless the matrix U specifying the Hamiltonian is diagonal. The transmission coefficient is "almost continuous" when the coupling constant g reaches the critical value $g = \frac{3}{4}$ above which H_1 is self-adjoint (cf.Remark 2.1) and the tunnelling is forbidden due to Theorem 3.3 of [I]. More explicitly, the relation (3.22a) holds with a possible exception of the "resonant" energies (3.22b) for which the tunnelling vanishes discontinuously at $g = \frac{3}{4}$. On the other hand, the barrier does not generally become fully transparent as $g \to 0+$, except for the special class of the matrices U specified above. This is not strange, however. Even for a very small g , the barrier still has the singularity at $x = 0$, which makes the motion over it different from the free-particle case.

References

A more complete list was given in [I] ; here we refer to :

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Диттрих Я., Экснер П. E2-84-353

Туннелирование сквозь сингулярный потенциальный барьер. Пример: $V(x) = gx^{-2}$

Продолжается обсуждение квантового туннелирования нерелятивистской частицы на прямой сквозь сингулярный потенциальный барьер V. В первой части этой работы мы показали, что если оператор $H_1 = -d^2/dx^2 + V(x)$ не является, по существу, самосопряженным, то туннелирование, в общем, не исключено и зависит от самосопряженного расширения оператора H_1, выбранного в качестве гамильтониана проблемы. Чтобы проиллюстрировать это явление, мы вычисляем коэффициент прохождения для всех самосопряженных расширений оператора H_1 соответствующего $V(x) = gx^{-2}$ при $0 < g < 3/4$.

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Dittrich J., Exner P. E2-84-353

Tunnelling Through a Singular Potential Barrier. An Example: $V(x) = gx^{-2}$

The study of quantum tunnelling of a non-reletivistic particle on the line through a singular potential barrier V is continued. In the first part of the paper, we have shown that if the operator $H_1 = -d^2/dx^2 + V(x)$ is not essentially self-adjoint on its natural domain, occurence of the tunnelling is not excluded, in general, and depends on the self-adjoint extension of H_1 we choose as Hamiltonian of the problem. In order to illustrate this phenomenon, we evaluate here the transmission coefficient for all self-adjoint extensions of the operator H_1 referring to $V(x) = gx^{-2}$ with $0 < g < 3/4$.

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

Communication of the Joint Institute for Nuclear Research. Dubna 1984