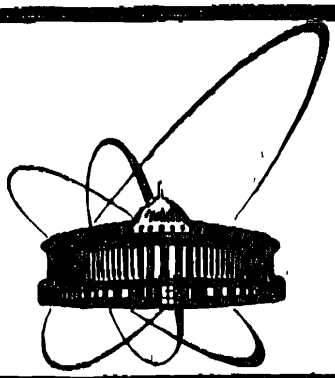

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QUANTUM MOTION ON A HALFLINE CONNECTED TO A PLANE

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1. Introduction

The theory of self-adjoint extensions represents a powerful heuristic way how to construct Hamiltonians of quantum systems in the cases when the correspondence principle yields an incomplete information only. For instance, Hamiltonians describing the point-interaction phenomena in quantum mechanics are obtained as self-adjoint extensions of the corresponding free Hamiltonians with the interaction points removed [1,2].

As another illustration, one can consider Schrödinger operators with singular potentials [3,4]. When the potential is singular enough, the correspondence principle provides us with a differential operator which is not essentially self-adjoint (e.s.a.). In this case, it is natural to approach the problem by constructing all self-adjoint extensions of this operator. After that one must select the appropriate one among them ; it requires, of course, an additional physical information. There are other quantum-mechanical problems to which the theory of self-adjoint extensions can be applied, e.g., a one-dimensional model of three-particle collisions [5].

Particularly interesting are the situations when a quantum particle moves on a spatial manifold which consists of several more simple parts. As an example, let us recall the free-electron (or metallic) model of organic molecules in which one assumes that the π-electrons move only along the graph Γ representing the molecule (cf., e.g., Ref.6 or Chap.6 of Ref.7 for the one-dimensional case). Suppose that the motion along the line Γ_j of Γ is described by the Hamiltonian

$$H_j = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V_j(x)$$

with a suitably chosen domain in $L^2(\Gamma_j,dx)$, where the coordinate x parametrizes $\Gamma_j \sim [0,l_j]$. The full Hamiltonian H of the model is now obtained as an appropriate self-adjoint extension of the operator

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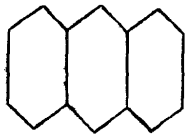

Fig.1. The graph Γ for an anthracene molecule.

constructed by "gluing together" the line Hamiltonians H_j.

The distinct parts of such a "configuration space" are not necessarily of the same dimension. In the present paper, we are going to discuss the most simple situation of this kind, where the manifold consists of a halfline attached to a plane, i.e., the dimensions are one and two, respectively. The motion in either part is assumed to be free. Notice that one may regard the sketched situation also as a motion in $\mathbb{R}^2$ subjected to a point interaction with some internal structure (compare to Ref.8). Such an interpretation, however, does not suit to the model we are going to discuss, for which analysis of the motion on the halfline is essential.

Let us resume briefly contents of the following sections. First of all, we construct the class of admissible Hamiltonians as self-adjoint extensions of the operator obtained by "gluing together" the free Hamiltonians for the motion on the halfline and the plane (Section 2). Since the direct characterization of these extensions obtained from the von Neumann's theory is not very suitable for practical calculations, we deduce in Section 3 an alternative classification of them using singular boundary conditions. In Section 4, we analyze the scattering on the point singularity, with a particular attention paid to the reflection coefficient for the particle travelling initially along the halfline. In conclusion, we discuss a possible application of the present analysis to modelling the quantum point-contact spectroscopy.

2. Admissible Hamiltonians

Let us consider a particle, an electron for definiteness, moving on the manifold G which consists of two parts - of the plane $\mathbb{R}^2$ and of the halfline $\mathbb{R}^- \equiv (-\infty, 0]$ which are connected at a point P as sketched on Fig.2 . The state Hilbert space of such a system is therefore orthogonal sum of the state spaces referring to the plane and to the halfline. If we neglect the possible internal degrees of freedom (spin of the electron, for instance), we have

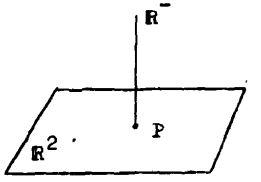

Fig.2. The manifold G.

$$\mathcal{H} = L^2(G) := L^2(\mathbb{R}^2) \oplus L^2(\mathbb{R}^-) . \qquad (1)$$

Since the electron motion is supposed to be free except at the point P , we start construction of Hamiltonian with the operator

$$H_0 = H_{0,1} \oplus H_{0,2} , \qquad (2)$$

where $H_{0,j}$ are restrictions of the respective free Hamiltonians on the two parts of G , namely

$$H_{0,1} = -\frac{d^2}{dx^2} , \qquad (3a)$$

$$D(H_{0,1}) = C_0^\infty(\mathbb{R}^- \setminus \{0\})$$

and

$$H_{0,2} = -\Delta , \qquad (3b)$$

$$D(H_{0,2}) = C_0^\infty(\mathbb{R}^2 \setminus \{P\}) .$$

The symbol $C_0^\infty(\Omega)$ denotes conventionally the set of all infinitely differentiable functions with a compact support contained in Ω .

The operator H_0 is not self-adjoint. It is well known[9] that the deficiency indices of $H_{0,1}$ are $(1,1)$, and the same is true for $H_{0,2}$ as we shall show a little later. Consequently, the deficiency indices of H_0 are $(2,2)$ so there is a four-parameter family of self-adjoint extensions. Let us construct them in detail.

We use the polar coordinates in the plane with the centre at P and decompose the space $L^2(\mathbb{R}^2)$ in the following way

$$L^2(\mathbb{R}^2) = L^2(\mathbb{R}^+, r\,dr) \otimes L^2(0,2\pi) = \bigoplus_{m=-\infty}^{\infty} L^2(\mathbb{R}^+, r\,dr) \otimes \{Y_m\}_{\mathrm{lin}} , \qquad (4)$$

where the functions

$$Y_m : \quad Y_m(\varphi) := (2\pi)^{-1/2}\, e^{im\varphi} , \quad \varphi \in [0,2\pi)$$

form the "trigonometric" orthonormal basis in $L^2(0,2\pi)$. Using the standard procedure (cf.Ref.9, appendix to Sec.X.1), one obtains the decomposition

$$H_{0,2} \restriction D_{min} = \bigoplus_{m=-\infty}^{\infty} h_m \otimes I \quad , \tag{5}$$

where

$$h_m = -\frac{d^2}{dr^2} - \frac{1}{r}\frac{d}{dr} + \frac{m^2}{r^2} \quad ,$$
$$D(h_m) = C_0^\infty(\mathbb{R}^+ \setminus \{0\}) \tag{6}$$

and the domain D_{min} consists of all finite linear combinations of the functions $\psi : \psi(r,\varphi) = f(r)Y_m(\varphi)$ with $f \in D(h_m)$. The deficiency indices of the operators h_m on $L^2(\mathbb{R}^+, r\,dr)$ are easily found. The latter are unitarily equivalent to

$$\tilde{h}_m = -\frac{d^2}{dr^2} + \frac{m^2 - \frac{1}{4}}{r^2}$$

on $D(\tilde{h}_m) = D(h_m)$, so we have

$$n(h_0) = 1 \quad ,$$
$$n(h_m) = 0 \quad \text{for} \quad m \neq 0 \quad . \tag{7}$$

The second relation follows from Theorem X.10 of Ref.9, while the first one verifies directly (a solution to the deficiency equations will be presented below). The relations (5) and (7) yield

$$n(H_{0,2}) \leq \sum_{m=-\infty}^{\infty} n(h_m) = 1 \quad . \tag{8a}$$

We want to show that equality holds in the last relation. To this end, one has to check that the functions $\psi_\pm : \psi_\pm(r,\varphi) = H_0^{(\alpha)}(\pm\sqrt{i}\,r)$, with α equal to 1,2 for the plus and minus sign, respectively, which span the deficiency subspaces (cf.(11) below) belong to $D(H_{0,2}^*)$. This can be performed in a straightforward manner using integration by parts and properties of the Hankel functions. The relation (2) then gives

$$n(H_0) = n(H_{0,1}) + n(H_{0,2}) = 2 \quad . \tag{8b}$$

Any self-adjoint extension of H_0 is therefore of the form

$$H = K \oplus \bar{h} \quad , \tag{9a}$$

where K is a self-adjoint extension of the operator K_0 on $L^2(\mathbb{R}^-) \oplus (L^2(\mathbb{R}^+, r\,dr) \otimes \{Y_0\})$ defined by

$$K_0 := H_{0,1} \oplus (h_0 \otimes I) \tag{9b}$$

and $\bar{h}$ denotes closure of the operator

$$h := \bigoplus_{\substack{m\in\mathbb{Z} \\ m\neq 0}} h_m \quad , \tag{9c}$$

which is e.s.a. due to (7).

Now we must choose suitable bases in the deficiency subspaces $\mathcal{K}_\pm = \mathrm{Ker}(K_0^* \mp iI)$. It is easy to find that $\mathcal{K}_+$ is spanned by the functions

$$\varphi_1^{(+)} = (f_1, 0) \quad , \quad \varphi_2^{(+)} = (0, f_2) \quad , \tag{10a}$$

where

$$f_1(x) := e^{\bar{\varepsilon}x} \quad , \quad \varepsilon = e^{\pi i/4} \quad ,$$
$$f_2(r) := (2\pi)^{1/2}\, H_0^{(1)}(\varepsilon r) \quad . \tag{11}$$

In the same way, the functions

$$\varphi_1^{(-)} = (\bar{f}_1, 0) \quad , \quad \varphi_2^{(-)} = (0, \bar{f}_2) \tag{10b}$$

form a basis in $\mathcal{K}_-$. The self-adjoint extensions of K_0 are now specified by isometries $\mathcal{K}_+ \to \mathcal{K}_-$, i.e., by 2×2 unitary matrices U . The von Neumann's theory gives a prescription how the extension K_U can be constructed for an arbitrary U : its domain $D(K_U)$ consists of all the functions which are of the form

$$f = \psi + c_1(\varphi_1^{(+)} + u_{11}\varphi_1^{(-)} + u_{12}\varphi_2^{(-)}) + c_2(\varphi_2^{(+)} + u_{21}\varphi_1^{(-)} + u_{22}\varphi_2^{(-)}), \tag{12}$$

with $\psi \in D(K_0)$ and $c_1, c_2 \in \mathbb{C}$, where u_{jk} are the elements of U . One might write down an expression for $K_U f$ as a linear combination of $K_0\psi$ and the deficiency functions. Instead, we are going to derive a more transparent expression for the action of K_U .

3. Boundary Conditions

For practical calculations, it is more convenient to characterize the extensions K_U by appropriate boundary conditions. In this way, we are able to describe K_U completely since $K_U \subset K_0^*$, and it is easy to see that

$$K_0^* f = \left\{ -\frac{d^2\varphi_1}{dx^2} \, , \, -\frac{d^2\varphi_2}{dr^2} - \frac{1}{r}\frac{d\varphi_2}{dr} \right\} \tag{13}$$

for each $f = \{\varphi_1, \varphi_2\}$ from $D(K_0^*)$. The deficiency functions $\varphi_2^{(\pm)}$ are, however, singular around P, but we can eliminate this difficulty by defining the regularized boundary values[10]

$$\begin{aligned} L_0(\varphi) &:= \lim_{r\to 0} \frac{\varphi(r)}{\ln r} \, , \\ L_1(\varphi) &:= \lim_{r\to 0} \left[\varphi(r) - L_0(\varphi) \ln r \right] \, , \end{aligned} \tag{14}$$

which will be used together with

$$\varphi_1(0_-) := \lim_{x\to 0-} \varphi_1(x) \, , \quad \varphi_1'(0_-) := \lim_{x\to 0-} \left(\frac{d}{dx}\varphi_1\right)(x) \, .$$

In particular, the standard expansions of Hankel functions[11] yield

$$\begin{aligned} L_0(f_2) &= -L_0(\bar{f}_2) = \frac{2i}{\pi} \, , \\ L_1(f_2) &= \frac{1}{2} + \frac{2i}{\pi}(\gamma - \ln 2) \, , \\ L_1(\bar{f}_2) &= \frac{1}{2} - \frac{2i}{\pi}(\gamma - \ln 2) \, , \end{aligned} \tag{15}$$

where $\gamma = 0.577216...$ is the Euler's constant.

Before proceeding further, we shall split the set of the matrices U characterizing the extensions into five disjoint classes :

Class I : contains all U such that $1 + u_{11} - u_{22} - \det U \neq 0$,

Class II : contains all non-diagonal U such that $1+u_{11}-u_{22}-\det U = 0$,

Class III : consists of the matrices $\begin{pmatrix} -1 & 0 \\ 0 & e^{i\omega} \end{pmatrix}$ with $\omega \in (0, 2\pi)$,

Clas IV : consists of the matrices $\begin{pmatrix} e^{i\omega} & 0 \\ 0 & 1 \end{pmatrix}$ with $\omega \in (-\pi, \pi)$,

Class V : contains the matrix $\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$.

Now we can formulate the mentioned result :

Theorem : Every self-adjoint extension of the operator H_0 is of the form $H_U := K_U \oplus \bar{h}$, where the operator K_U is specified uniquely by the following boundary conditions. If $f = \{\varphi_1, \varphi_2\}$ belongs to $D(K_U)$, then

(i) for U of the class I, we have

$$\begin{aligned} \varphi_1'(0_-) &= A\varphi_1(0_-) + BL_0(\varphi_2) \, , \\ L_1(\varphi_2) &= C\varphi_1(0_-) + DL_0(\varphi_2) \, , \end{aligned} \tag{16a}$$

where the coefficients are related to the matrix elements of U by

$$A = \frac{\bar{\varepsilon}(1 - u_{22}) + \varepsilon(u_{11} - \det U)}{1 + u_{11} - u_{22} - \det U} \, , \tag{16b}$$

$$B = \frac{\pi}{\sqrt{2}} \frac{u_{21}}{1 + u_{11} - u_{22} - \det U} \, , \tag{16c}$$

$$C = \frac{u_{12}}{1 + u_{11} - u_{22} - \det U} \, , \tag{16d}$$

$$D = \gamma - \ln 2 + \frac{\pi}{4i} \frac{1 + u_{11} + u_{22} + \det U}{1 + u_{11} - u_{22} - \det U} \, , \tag{16e}$$

(ii) if U belongs to the class II, then

$$\begin{aligned} L_0(\varphi_2) &= E\varphi_1(0_-) \, , \\ L_1(\varphi_2) &= F\varphi_1(0_-) + G\varphi_1'(0_-) \, , \end{aligned} \tag{17a}$$

where

$$E = \frac{2i}{\pi} \frac{1 - u_{22}}{u_{21}} = -\frac{2i}{\pi} \frac{u_{12}}{1 + u_{11}} \, , \tag{17b}$$

$$F = \frac{i}{\sqrt{2}\, u_{21}} \left\{ \bar{\varepsilon} + \varepsilon u_{11} + i\sqrt{2}\,(1-u_{22}) L_1(\bar{f}_2) \right\} \, , \tag{17c}$$

$$G = -\frac{i}{\sqrt{2}} \frac{1 + u_{11}}{u_{21}} \, , \tag{17d}$$

(iii) for U of the class III, the boundary conditions read

$$\begin{aligned} \varphi_1(0_-) &= 0 \, , \\ L_1(\varphi_2) &= \frac{\pi}{4} \left(\operatorname{ctg} \frac{\omega}{2}\right) L_0(\varphi_2) \, , \end{aligned} \tag{18}$$

(iv) if U belongs to the class IV, we have

$$\varphi_1'(0_-) = \frac{1}{\sqrt{2}}(1 - \mathrm{tg}\,\tfrac{\omega}{2})\,\varphi_1(0_-) \quad , \qquad (19)$$

$$L_0(\varphi_2) = 0 \quad ,$$

(v) finally, if $U = \begin{matrix} -1 & 0 \\ 0 & 1 \end{matrix}$, then

$$\varphi_1(0_-) = L_0(\varphi_2) = 0 \quad . \qquad (20)$$

Proof : Suppose first that U belongs to the class I. We express φ_1, φ_2 from (12) and insert into (16a) ; it yields the equations

$$\bar{\varepsilon} + u_{11}\varepsilon = A(1+u_{11}) + Bu_{12}L_0(\bar{f}_2) \quad ,$$

$$u_{12}\varepsilon = Au_{21} + B\left[L_0(f_2) + u_{22}L_0(\bar{f}_2)\right] \quad ,$$

$$u_{12}L_1(\bar{f}_2) = C(1+u_{11}) + Du_{12}L_0(\bar{f}_2) \quad ,$$

$$L_1(f_2) + u_{22}L_1(\bar{f}_2) = Cu_{21} + D\left[L_0(f_2) + u_{22}L_0(\bar{f}_2)\right] \quad .$$

Now we substitute from (15), then the solution for $1 + u_{11} - u_{22} - \det U \neq 0$ is given by (16b-e). In a similar way, one obtains the relations (17)-(20).

Next one has to check that the mapping from the set of matrices U to the set of boundary conditions is injective. This is easy for the classes III-V . Assume further that there are U, U' of the class II both leading to the conditions (17), i.e., $E = E'$, etc. Then we have $G/E = G'/E'$ and $F/E = F'/E'$ so

$$\frac{1+u_{11}}{1-u_{22}} = \frac{1+u'_{11}}{1-u'_{22}} \quad \text{and} \quad \frac{\bar{\varepsilon}+\varepsilon u_{11}}{1-u_{22}} = \frac{\bar{\varepsilon}+\varepsilon u'_{11}}{1-u'_{22}} \quad .$$

Now one has to multiply the second equation by $\bar{\varepsilon}$ and to subtract it from the first one. It yields $u_{22} = u'_{22}$. Substituting this back to the first equation, we get $u_{11} = u'_{11}$. Finally, the relations $u_{jk} = u'_{jk}$ for $jk = 12, 21$ follow from (17b) ; one has to notice that $|u_{jj}| < 1$ since U is unitary and non-diagonal.

The argument is most complicated for class I . Assume again that there are U, U' which yield the same values of the coefficients (16b-e). Then we have

$$\frac{u_{jk}}{1+u_{11}-u_{22}-\det U} = \frac{u'_{jk}}{1+u'_{11}-u'_{22}-\det U'} \qquad (21)$$

for $jk = 12$ and 21 . Moreover, the relations (16e) and (16b) after substituting for ε give

$$\frac{1 \pm u_{11} \pm u_{22} + \det U}{1+u_{11}-u_{22}-\det U} = \frac{1 \pm u'_{11} \pm u'_{22} + \det U'}{1+u'_{11}-u'_{22}-\det U'} \quad .$$

It further implies

$$1 + u_{11} = \alpha(1+u'_{11}) \quad ,$$

$$1 - u_{22} = \alpha(1-u'_{22}) \quad , \qquad (22a)$$

where we have denoted

$$\alpha = \frac{1+u_{11}-u_{22}-\det U}{1+u'_{11}-u'_{22}-\det U'} \quad . \qquad (23)$$

The relations (21) can be similarly rewritten as

$$u_{12} = \alpha u'_{12} \quad , \quad u_{21} = \alpha u'_{21} \quad . \qquad (22b)$$

Hence $(1+u_{11})(1-u_{22}) + u_{12}u_{21} = \alpha^2\left[(1+u'_{11})(1-u'_{22}) + u'_{12}u'_{21}\right]$, and combining this relation with (23), we get $\alpha^2 = \alpha$. Since α is non-zero by assumption, we obtain $\alpha = 1$; then $U = U'$ follows from (22). ∎

In this way, we have been able to characterize the operators H_U by means of the boundary conditions. The relations (16b-e),(17b-d) do not show explicitly which values the coefficients may assume. It becomes more clear, if one uses a suitable parametrization of the matrix U , such as (29) below.

4. Scattering on the Singularity

Now we are going to discuss the extensions H_U , with a particular attention paid to scattering on the singular point P . We shall distiguish two cases :

(a) U diagonal : going through the boundary conditions (16),(18)--(20), one finds easily that they separate. We can express them in the form

$$\varphi_1'(0_-) = A\varphi_1(0_-) \quad , \tag{24a}$$

$$L_1(\varphi_2) = DL_0(\varphi_2) \quad , \tag{24b}$$

where the coefficients are with the usual license written as

Class I : $A = \frac{\bar{\varepsilon} + \varepsilon u_{11}}{1 + u_{11}}$, $D = \gamma - \ln 2 + \frac{\pi}{4i}\frac{1 + u_{22}}{1 - u_{22}}$

(notice that both A and D are real ; this remains true for non-diagonal matrices U - cf.(30a,d) below)

Class III : $A = \infty$, $D = \frac{\pi}{4}\operatorname{ctg}\frac{\omega}{2}$

Class IV : $A = \frac{1}{2}(1 - \operatorname{tg}\frac{\omega}{2})$, $D = \infty$

Class V : $A = D = \infty$.

Hence the system separates for a diagonal U into two independent subsystems and its Hamiltonian is of the form

$$H_U = H_{0,1}^{(A)} \oplus H_{0,2}^{(D)} \quad , \tag{25}$$

where $H_{0,1}^{(A)}$ is the halfline Hamiltonian (cf.Ref.9, Sec.X.1) specified by (24a) and $H_{0,2}^{(D)} = h_0^{(D)} \oplus \bar{h}$ is the two-dimensional point-interaction Hamiltonian (cf.Ref.12). Scattering by this point interaction as well as reflection on the halfline should be considered separately ; passage of the electron between the two parts of the configuration manifold is impossible.

(b) U non-diagonal : now the transitions from $\mathbb{R}^-$ to $\mathbb{R}^2$ and vice versa become possible. First of all, we shall discuss in detail the situation when U belongs to the class I . Let us consider reflection of the electron moving initially along the halfline towards P . Using the boundary conditions (16), it is easy to see that the function $f_U = (\varphi_1^U, \varphi_2^U)$ with

$$\varphi_1^U(x) = e^{ikx} + a_U e^{-ikx} \quad , \tag{26a}$$

$$\varphi_2^U(r) = \tilde{b}_U H_0^{(1)}(kr) \tag{26b}$$

for a given $k > 0$ belongs locally to $D(H_U)$ if

$$a_U = -\frac{(A - ik)\left[1 + \frac{2i}{\pi}(\gamma - D + \ln\frac{k}{2})\right] + \frac{2i}{\pi}BC}{(A + ik)\left[1 + \frac{2i}{\pi}(\gamma - D + \ln\frac{k}{2})\right] + \frac{2i}{\pi}BC} \quad , \tag{27a}$$

$$\tilde{b}_U = \frac{2iCk}{(A + ik)\left[1 + \frac{2i}{\pi}(\gamma - D + \ln\frac{k}{2})\right] + \frac{2i}{\pi}BC} \quad . \tag{27b}$$

Moreover, it holds

$$(-\frac{d^2}{dx^2} - k^2)\varphi_1^U = 0 \quad ,$$

$$(-\Delta - k^2)\varphi_2^U = 0 \quad ,$$

so f_U given by the relations (26) and (27) is a generalized eigenvector of H_U , and $|a_U|^2$ is therefore nothing but the reflection coefficient at the point singularity.

The relation (27a) shows that the reflection coefficient depends on the chosen Hamiltonian H_U . In particular, $|a_U| = 1$ holds if U becomes diagonal so $BC = 0$; the electron can be then only reflected at P . On the other hand, occurrence of the transition from $\mathbb{R}^-$ to $\mathbb{R}^2$ means

$$|a_U| < 1 \quad . \tag{28a}$$

We shall check directly that this inequality holds once U is non-diagonal. To this end, we shall use the following explicit parametrization of a unitary 2×2 matrix

$$U = e^{i\xi}\begin{pmatrix} e^{i(\alpha+\delta)}\cos\beta & e^{i(\delta-\alpha)}\sin\beta \\ -e^{i(\alpha-\delta)}\sin\beta & e^{-i(\alpha+\delta)}\cos\beta \end{pmatrix} \quad , \tag{29}$$

where $\alpha, \beta, \delta, \xi$ are real parameters (the first three of them are nothing but doubled Euler angles). It yields the following expressions for the coeffients (16b-e) :

$$A = \frac{\mathcal{Y}}{\mathcal{D}} \quad , \tag{30a}$$

$$B = \frac{\pi i}{2\sqrt{2}}\frac{e^{i(\alpha-\delta)}\sin\beta}{\mathcal{D}} \quad , \tag{30b}$$

$$C = -\frac{i}{\sqrt{2}}\frac{e^{i(\delta-\alpha)}\sin\beta}{\mathcal{D}} \quad , \tag{30c}$$

$$D = \gamma - \ln 2 - \frac{\pi}{4}\frac{\mathcal{C}}{\mathcal{D}} \quad , \tag{30d}$$

where

$$\mathcal{Y} = \sin(\alpha + \delta + \tfrac{\pi}{4})\cos\beta - \sin(\xi + \tfrac{\pi}{4}) \quad ,$$

$$\mathcal{D} = \sin(\alpha+\delta)\cos\beta - \sin\xi \ ,$$

$$\mathcal{C} = \cos(\alpha+\delta)\cos\beta + \cos\xi \ ;$$

notice that $\mathcal{D}$ is non-zero for the class I matrices. As we have remarked, the relations (30) show that the "diagonal" coefficients A,D are real-valued, while the "non-diagonal" ones are complex conjugated up to a real multiplicative constant. Using these expressions, we find

$$a_U = -\frac{(\mathcal{J}-ik\mathcal{D})\left[(1+\frac{2i}{\pi}\ln k)\mathcal{D}+\frac{1}{2}\mathcal{C}\right]+\frac{i}{2\sqrt{2}}\sin^2\beta}{(\mathcal{J}+ik\mathcal{D})\left[(1+\frac{2i}{\pi}\ln k)\mathcal{D}+\frac{1}{2}\mathcal{C}\right]+\frac{i}{2\sqrt{2}}\sin^2\beta} \qquad (31)$$

so after a short calculation we arrive at the relation

$$1-|a_U|^2 = \qquad (28b)$$

$$= \frac{\sqrt{2}\mathcal{D}^2 k\sin^2\beta}{\mathcal{D}^2(\mathcal{J}-\frac{2}{\pi}\mathcal{D}k\ln k-\frac{1}{2}\mathcal{C}k)^2+(\frac{1}{2}\mathcal{J}\mathcal{C}+\frac{2}{\pi}\mathcal{J}\mathcal{D}\ln k+\mathcal{D}^2k+\frac{1}{2\sqrt{2}}\sin^2\beta)^2} > 0 \ ,$$

which proves (28a).

Notice that the squared modulus of (27b) is not the transition coefficient, since it is not properly normalized. The relation (28b) shows that it is $b_U = (\sqrt{2}/k)^{1/2}\tilde{b}_U$ which fulfils $|a_U|^2+|b_U|^2 = 1$.

The fact that the singularity is penetrable for a non-diagonal U can be seen also when one considers scattering of the electron moving in the plane at the point P . The corresponding generalized eigenfunction is $f_U = (\psi_1^U, \psi_2^U)$ with

$$\psi_1^U(x) = \tilde{c}_U e^{-ikx} \ , \qquad (32a)$$

$$\psi_2^U(r) = J_0(kr) + d_U H_0^{(1)}(kr) \ , \qquad (32b)$$

where

$$\tilde{c}_U = \frac{2i}{\pi}\frac{B}{(A+ik)\left[1+\frac{2i}{\pi}(\mathcal{J}-D+\ln\frac{k}{2})\right]+\frac{2i}{\pi}BC} \ , \qquad (33a)$$

$$d_U = -\frac{1}{1+\frac{2i}{\pi}(\mathcal{J}-D+\ln\frac{k}{2}+\frac{BC}{A+ik})} \qquad (33b)$$

if we require f_U to belong locally to $D(H_U)$. The asymptotics for large r can be found easily,

$$\psi_2^U(r) = \left(\frac{2}{\pi kr}\right)^{1/2} e^{i\delta_0(k)}\sin(kr+\frac{\pi}{4}+\delta_0(k)) + O(r^{-1}) \ , \qquad (34)$$

where $\delta_0(k)$ is given by

$$S_0(k) = e^{2i\delta_0(k)} = \frac{\mathcal{J}-D+\ln\frac{k}{2}+\frac{\pi i}{2}+\frac{BC}{A+ik}}{\mathcal{J}-D+\ln\frac{k}{2}-\frac{\pi i}{2}+\frac{BC}{A+ik}} \ . \qquad (35a)$$

Here $\delta_0(k)$ represents the s-wave scattering phase shift and $S_0(k)$ is the on-shell s-wave scattering matrix. For the higher partial waves, we get

$$\delta_m(k) = 0 \quad , \quad m = \pm1, \pm2, \ldots \ . \qquad (35b)$$

In general, the scattering matrix is not unitary. This is not surprising, because the electron can continue its motion in $\mathbb{R}^2$ after the scattering, vanishing thus from the plane. In order to demonstrate it explicitly, one has to express $S_0(k)$ using the parametrization (29). A short calculation then gives

$$1-|S_0(k)|^2 = 1-|a_U|^2 \ , \qquad (36)$$

where the rhs is given by (28b). Hence S is non-unitary iff U is non-diagonal.

Let us turn now to matrices U of the class II . In this case, too, the electron is able to pass through the singular point. The analysis is essentially the same as above. We restrict ourselves with presenting the results. For the generalized eigenvector (26), we find now

$$a_U = -\frac{1+\frac{2i}{\pi}(\mathcal{J}-\frac{F+ikG}{E}+\ln\frac{k}{2})}{1+\frac{2i}{\pi}(\mathcal{J}-\frac{F-ikG}{E}+\ln\frac{k}{2})} \ , \qquad (37a)$$

$$\tilde{b}_U = \frac{2ikG}{1+\frac{2i}{\pi}(\mathcal{J}-\frac{F-ikG}{E}+\ln\frac{k}{2})} \ . \qquad (37b)$$

On the other hand, for the scattering in the plane corresponding to (32), one can find the coefficients $\tilde{c}_U, d_U$, which give

$$S_0(k) = e^{2i\delta_0(k)} = \frac{\mathcal{J}-\frac{F-ikG}{E}+\frac{\pi i}{2}+\ln\frac{k}{2}}{\mathcal{J}-\frac{F-ikG}{E}-\frac{\pi i}{2}+\ln\frac{k}{2}} \ . \qquad (38)$$

5. A Possible Application

The problem treated in the preceding sections may seem somewhat bizarre. Nevertheless, it can have a quite reasonable physical application as a model of the quantum point-contact spectroscopy.

For a metallic contact, one usually expects a linear relation between the applied voltage and the current according to Ohm's law. This is true if the size of the contact is large enough. On the other hand, if its linear dimension becomes comparable with mean free path of the electrons in metal, then interesting non-linear effects in the current-voltage characteristics can be observed - cf.Ref.13 for a review. In this case, the electrons are scattered at the orifice giving rise to a backward flow, which adds a negative and voltage-dependent contribution to the current.

The results of the present analysis can be used for modelling such a contact whose linear dimension tends to zero. In order to calculate the current through the contact[14], one has to know the electron-gas density and the transmission coefficient through the singular point. In the simplest case, when the electrons are supposed to be free, the latter is given by (28b) (or an analogous expression for U of the class II). If we add a potential to H_U which should describe the metallic structure of the system (a wire connected to a thin plate), then the transmission coefficient must be calculated anew. It remains possible, however, to characterize the admissible Hamiltonians by the boundary conditions listed in the theorem of Section 3, as far as the potential is bounded.

We are going to discuss the model, which we have sketched briefly here, in a subsequent paper.

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Экснер П., Шеба П.

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Квантовое движение на полупрямой присоединенной к плоскости

В настоящей работе рассматривается свободное движение частицы на многообразии, состоящем из одномерной и двумерной частей. При помощи теории самосопряженных расширений найден класс допустимых гамильтонианов. Внимание уделено, в частности, тем из них, которые допускают проход частицы сквозь точечную сингулярность; вычислен коэффициент отражения и другие величины, характеризующие рассеяние. Обсуждается возможное физическое применение.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Сообщение Объединенного института ядерных исследований. Дубна 1986

Exner P., Šeba P.

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Quantum Motion on a Halfline Connected to a Plane

In this paper, we treat free motion of a particle on a manifold which consists of a one-dimensional and a two-dimensional parts connected in one point. The class of admissible Hamiltonians is found using the theory of self-adjoint extensions. A particular attention is paid to those of them which allow the particle to pass through the point singularity; we calculate the reflection coefficient and other quantities characterizing scattering on the connection point. A possible application is discussed.

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

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