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A SIMPLE MODEL OF THIN-FILM POINT CONTACT IN TWO AND THREE DIMENSIONS

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1. Introduction

The theory of self-adjoint extensions is a part of functional analysis which is commonly regarded as classical. Recently, it has attracted a new interest connected with applications in quantum physics which include, e.g., rigorous treatment of point interactions[1-8], a model of three-particle resonances[9], the so-called metallic models of molecules[10], some properties of singular potentials such as tunneling effect in one dimension[11] or various regularization procedures[12-14], etc.

The theory of self-adjoint extension gives us also a possibility to construct models describing experiments in the quantum point-contact spectroscopy, where one studies deviations from the Ohm's law on metallic contacts whose diameter is small comparing to the mean free path of the electrons in metal[15]. In a recent series of papers[16-18], we have analyzed very simple models, in which the electrons are supposed to be free and spinless, for two typical situations usually dubbed spear-and-anvil contact and thin-film contact. Despite their simplicity, the models are able to reproduce the basic non-linear shape of the observed current-voltage characteristics of the "point" contacts as we have illustrated on examples in Ref.18. On the other hand, one cannot obtain in this way the fine structure of the current-voltage characteristics, which is not surprising, because we have neglected completely structure of the metal (which might be modelled by adding a suitable periodic potential). Another open question concerns the choice of the right self-adjoint extension which should play the role of Hamiltonian; one would invite a choice guided by some physical considerations rather than a fit to experimental data.

Before dealing with these problems, however, one must analyze basic features of this class of models. The present paper is a part of this program : we concentrate our attention here to the problem how the current-voltage characteristic of a thin-film contact is influen-

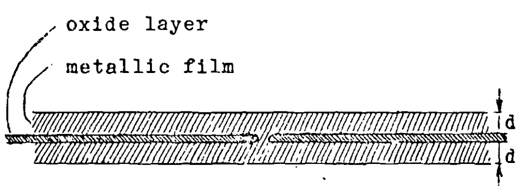

Fig.1. Scheme of the point-contact experiment with thin films.

ced by thickness of the metallic films. A typical experiment is sketched schematically on Fig.1. Two metallic films are produced on a substrate by an evaporation technique, separated by a very thin oxide layer in which a crack is produced by an electric breakdown or mechanically. It is well known from the pioneering experiments [19] that the current-voltage characteristic at low energies exhibits oscillations whose frequency is inversely proportional to the thickness d of the films.

We are going to discuss two extreme situations. In the first of them, the film is supposed to be very thick, i.e., $d=\infty$; then we have to analyze motion of a particle in two halfspaces separated by a plane with one point "hole". One must choose, of course, suitable boundary conditions on this plane. Since we have in mind motion of electrons in metal, the Neumann condition is an appropriate choice. Other possibilities are discussed in Section 3 ; in particular, we show there that one cannot construct a model of this type, in which the electron is allowed to pass from one halfspace to the other, with Dirichlet condition.

Starting from the free Hamiltonian in halfspace, we construct a four-parameter family of self-adjoint extensions H_U which may be used as Hamiltonians for a (spinless) electron moving on the described configuration manifold ; each of them is characterized by suitable singular boundary conditions at the point connecting the halfspaces. Among the admissible Hamiltonians, there is a physically interesting two-parameter family containing the operators commuting with the modified parity operator which exchanges the halfspaces. In Section 6, we calculate the transmission coefficient for each of the operators H_U .

The second extreme is represented by the situation, when the film is very thin so one can set $d=0$. The configuration manifold can be modelled in this case by two planes connected at one point. This problem has been discussed in Ref.17 ; in Section 7, we rewrite the boundary conditions obtained there in a more convenient way and calculate

the transmission coefficient. Since it yields easily the current-voltage characteristics, we are able to compare results for the two situations. This is done in the concluding section ; the result is that for thin films, the observed deviations from the Ohm's law are (at least, in part) a global quantum (or geometrical) effect rather than a consequence of the electron-phonon interaction.

2. The Operator h_0

Consider first the Laplacian in halfspace specified by the Neumann boundary condition, i.e., the operator h on $L^2(\mathbb{R}^2\times\mathbb{R}_+)$ defined by

$$h\psi = -\Delta\psi \tag{2.1a}$$

with

$$D(h) = \{\psi\in L^2(\mathbb{R}^2\times\mathbb{R}_+) : \Delta\psi\in L^2(\mathbb{R}^2\times\mathbb{R}_+) \text{ in the sense of distributions, } \frac{\partial}{\partial x_3}\psi(x)\Big|_{x_3=0} = 0\} . \tag{2.1b}$$

Points of $\mathbb{R}^2\times\mathbb{R}_+$ are denoted as $x=(x_1,x_2,x_3)$ with $x_1,x_2\in\mathbb{R}$ and $x_3\in\mathbb{R}_+$.

The operator h is self-adjoint. Our construction will start from its non-selfadjoint restriction

$$h_0 := h\restriction D_0 , \tag{2.2a}$$

$$D(h_0) = \{\psi\in D(h) : \psi(x)=0 \text{ for } x \text{ of some neighborhood of the point } 0\} . \tag{2.2b}$$

Let us look for the deficiency indices of h_0 . It is useful to work in the spherical coordinates with the center at 0 ,

$$x_1 = r\sin\vartheta\cos\varphi , \quad x_2 = r\sin\vartheta\sin\varphi , \quad x_3 = r\cos\vartheta , \tag{2.3}$$

where $r\in\mathbb{R}_+$, $\varphi\in[0,2\pi)$ and $\vartheta\in[0,\frac{\pi}{2}]$. The Hilbert space decomposes conventionally as

$$L^2(\mathbb{R}^2\times\mathbb{R}_+) = L^2(\mathbb{R}_+,r^2dr)\otimes L^2(S_+^{(2)},d\Omega) , \tag{2.4}$$

where $S_+^{(2)}$ is the halfsphere of unit radius and $d\Omega$ the rotationally invariant measure on it. The operator h can be rewritten in the coordinates (2.3) as

$$hf = -\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial f}{\partial r}\right) + \frac{1}{r^2}\Lambda f \ , \qquad (2.5a)$$

where Λ is the modified squared angular momentum operator defined by the differential expression

$$\Lambda = -\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\,\frac{\partial}{\partial\vartheta}\right) - \frac{1}{\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2} \qquad (2.5b)$$

together with the boundary condition

$$\frac{\partial}{\partial\vartheta} f(\vartheta,\varphi)\Big|_{\vartheta=\pi/2} = 0 \qquad (2.5c)$$

which follows from the Neumann condition in (2.1b).

2.1 Proposition : Λ has a purely point spectrum, $\Lambda f_{lm} = l(l+1)f_{lm}$, $l=0,1,2,\dots$, $m=-l,-l+2,\dots,l$, where $f_{lm} = Y_{lm}\restriction S_+^{(2)}$ with $l+m$ even.

Proof : It is easy to see that f_{lm} are eigenvectors of Λ . It remains to check that they span the space $L^2(S_+^{(2)})$. Suppose that a function $g\in L^2(S_+^{(2)})$ fulfils

$$\int_0^{\pi/2}\sin\vartheta\,d\vartheta\int_0^{2\pi}d\varphi\,\overline{g(\vartheta,\varphi)}f_{lm}(\vartheta,\varphi) = 0 \qquad (2.6a)$$

for all $l=0,1,2,\dots$ and $m=-l,-l+2,\dots,l$. We extend g to the sphere $S^{(2)}$ by

$$\tilde g(\vartheta,\varphi) := \begin{cases} g(\vartheta,\varphi) & \dots\ 0\le\vartheta\le\pi/2 \\ g(\pi-\vartheta,\varphi) & \dots\ \pi/2<\vartheta\le\pi \end{cases}$$

so $\tilde g$ is an even function with respect to $\vartheta\to\pi-\vartheta$ (with a possible exception of a zero measure set). It holds $Y_{lm}(\pi-\vartheta,\varphi) = (-1)^{l+m}Y_{lm}(\vartheta,\varphi)$, and therefore (2.6a) gives

$$\int_0^{\pi}\sin\vartheta\,d\vartheta\int_0^{2\pi}d\varphi\,\overline{\tilde g(\vartheta,\varphi)}Y_{lm}(\vartheta,\varphi) = 0 \qquad (2.6b)$$

for $l+m$ even ; the same relation holds trivially for $l+m$ odd. Since $\{Y_{lm}\}$ forms an orthonormal basis in $L^2(S^{(2)})$, it follows that $\tilde g = 0$, i.e., $g=0$. ∎

We denote further by $\mathcal{K}_l$ the eigenspaces $\mathrm{lin}\{f_{lm} : m=-l,-l+2,\dots,l\}$; then the Hilbert space (2.4) decomposes as

$$L^2(\mathbb{R}^2\times\mathbb{R}_+) = \bigoplus_{l=0}^{\infty} L_l \ , \qquad (2.7a)$$

where

$$L_l = L^2(\mathbb{R}_+, r^2dr)\otimes\mathcal{K}_l \qquad (2.7b)$$

and for h we obtain

$$h = \bigoplus_{l=0}^{\infty} h^{(l)}\otimes I \ , \qquad (2.8)$$

where

$$h^{(l)}f = -\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{df}{dr}\right) + \frac{l(l+1)}{r^2}f \qquad (2.9a)$$

with

$$D(h^{(l)}) = \{f\in L^2(\mathbb{R}_+, r^2dr) : f,f'\in AC[\mathbb{R}_+] \text{ and } h^{(l)}f\in L^2(\mathbb{R}_+, r^2dr)\} \ . \qquad (2.9b)$$

In the same way, we get the expansion of h_0 :

$$h_0 = \bigoplus_{l=0}^{\infty} h_0^{(l)}\otimes I \ , \qquad (2.10)$$

where $h_0^{(l)}$ is again given by the rhs of (2.9a) and

$$D(h_0^{(l)}) = \{f\in D(h^{(l)}) : f(r)=0 \text{ on some neighborhood of } 0\} \qquad (2.11)$$

Hence the self-adjointness problem for h_0 is reduced to analysis of the operators $h_0^{(l)}$. They are e.s.a. for $l\ge 1$ (cf. Theorem X.10 of Ref.20), while $h_0^{(0)}$ can be easily seen to have the deficiency indices equal to (1,1) - solution to the deficiency equations will be presented below. Consequently, we have.

2.2 Proposition : The deficiency indices of h_0 are (1,1) .

Before using this information, we are going to make a short digression concerning a more general type of boundary conditions.

3. The Mixed Boundary Conditions

If we replace the Neumann boundary condition in (2.1b) by the Dirichlet one, the corresponding operator h_0 will be e.s.a. In order to see this, one has to realize that the modified squared angular momentum operator Λ is specified in this case by the boundary condition $f(\pi/2,\varphi) = 0$ instead of (2.5c). An argument similar to proof of Proposition 2.1 then shows that it has a pure point spectrum, $\Lambda f_{lm} = l(l+1)f_{lm}$, where now $f_{lm} = Y_{lm} \upharpoonright S_+^{(2)}$ with $l+m$ odd. It means that $l = 1,2,\ldots$ and all terms in the decomposition analogous to (2.10) are e.s.a.

These boundary conditions represent particular cases of a more general condition of the mixed type, namely

$$\frac{\partial}{\partial x_3}\psi(x)\Big|_{x_3=0} = \frac{c}{r}\psi(x) \quad , \tag{3.1a}$$

where c is a real number. In the spherical coordinates, this condition is independent of r and looks as follows

$$-\frac{\partial}{\partial\vartheta} f(\vartheta,\varphi)\Big|_{\vartheta=\pi/2} = c\, f(\pi/2,\varphi) \quad . \tag{3.1b}$$

The condition (3.1) can be interpreted as adding a surface-interaction term which is repulsive (with respect to the origin) if $c > 0$ and attractive for $c < 0$. The Dirichlet condition corresponds to the case of infinitely strong repulsion, while the Neumann one means that the surface term is absent. Somewhere between them there is a critical point c_{nsa} in which the repulsin becomes weak enough that the operator h_0 ceases to be e.s.a., i.e., the deficiency indices jump from (0,0) to (1,1) - cf.Fig.2 . There is another critical point in which the attraction becomes so strong that the particle can collapse into the singularity, i.e., the spectrum of h_0 is unbounded from below.

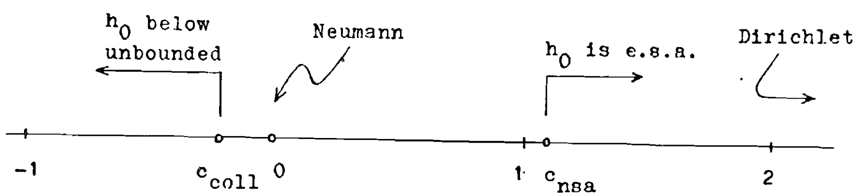

Fig.2. The critical values of the boundary condition (3.1).

The aim of this section is to find the above named critical points. In the same way as above, one can decompose h_0 into an orthogonal sum, and to reduce therefore the problem to analysis of the operators

$$h_0^{(\nu)} : h_0^{(\nu)} f = -\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{df}{dr}\right) + \frac{\nu(\nu+1)}{r^2} f \tag{3.2a}$$

with

$$D(h_0^{(\nu)}) = \left\{ f\in L^2(\mathbb{R}_+,r^2dr) : f,f' \in AC[\mathbb{R}_+], f(r)=0 \text{ in some neighborhood of } 0 \text{ and } h_0^{(\nu)} f \in L^2(\mathbb{R}_+,r^2dr) \right\} . \tag{3.2b}$$

The numbers $\nu(\nu+1)$ are obtained by solving the eigenvalue problem

$$\Lambda f_{\nu m} = \nu(\nu+1) f_{\nu m} \tag{3.3}$$

for the modified squared angular momentum operator, which is now given by the expression (2.5b) together with the boundary condition (3.1b) (at the same time, of course, one must demand the functions $f_{\nu m}$ to be regular at the pole ($\vartheta = 0$)). Conventionally, we substitute $f_{\nu m}(\vartheta,\varphi) = g(\cos\vartheta)\, e^{im\varphi}$ for $m = 0,\pm1,\pm2,\ldots$ obtaining in this way the eigenvalue problem for the ordinary differential operator

$$L_m : L_m g = (z^2-1)g'' + 2zg' + \frac{m^2}{1-z^2} g \quad , \tag{3.4a}$$

i.e., the Legendre equation, with the boundary conditions

$$g \text{ regular at } z = 1 \qquad g'(0) = cg(0) \tag{3.4b}$$

In distinction to the particular cases $c = 0,\infty$, **the solution to (3.3) need** not generally exhibit degeneracy with respect to m ; only the degeneracy with respect to the sign of m persists. Hence for each $m = 0,\pm1,\pm2,\ldots$, we have a sequence of values $\nu(\nu+1)$ which obey (3.3). The equation $L_m g = \nu(\nu+1)g$ is solved by the first-order Legendre function $g(z) = P_\nu^m(z)$; the solution Q_ν^m is excluded by the first one of the conditions (3.4b) - cf.Ref.21, 8.711.4 . The second condition leads to the equation

$$2\,\mathrm{tg}\left[\frac{\pi}{2}(\nu+m)\right] = c\,\frac{\Gamma(\frac{1}{2}\nu+\frac{1}{2}m+\frac{1}{2})\Gamma(\frac{1}{2}\nu-\frac{1}{2}m+\frac{1}{2})}{\Gamma(\frac{1}{2}\nu+\frac{1}{2}m+1)\Gamma(\frac{1}{2}\nu-\frac{1}{2}m+1)} \tag{3.5}$$

(cf.Ref.22, 8.6) ; solving it for ν one can obtain the eigenvalues of (3.3).

Fortunately, it is not necessary to perform the task in the general setting. As we have mentioned, the operator $h_0^{(\nu)}$ is e.s.a. iff $\nu(\nu+1)\geq\frac{3}{4}$. It is also well known (see, e.g., Ref.23) that $h_0^{(\nu)}$ is bounded from below iff $\nu(\nu+1)\geq-\frac{1}{4}$. Hence the lowest eigenvalue in (3.3) is decisive for both of our problems. It is an easy consequence of the minimax principle (Ref.20, Theorem XIII.1) that the "ground states" of L_m are not lower than that of L_0 , i.e., $\inf\sigma(L_0)\leq\inf\sigma(L_m)$ for each m . It is therefore sufficient to solve the equation (3.5) for m=0 when it acquires the form

$$2\,\mathrm{tg}\left(\frac{\pi}{2}\nu\right)=c\left(\frac{\Gamma(\frac{1}{2}\nu+\frac{1}{2})}{\Gamma(\frac{1}{2}\nu+1)}\right)^2 \quad . \tag{3.6a}$$

The eigenvalue $\nu(\nu+1)$ has to be real so ν is either real belonging to $[-\frac{1}{2},\infty)$ or $\nu=-\frac{1}{2}+i\beta$ with $\beta\in\mathbb{R}$. The rhs of (3.6a) is a monotonous function of ν in $[-\frac{1}{2},\infty)$ (decreasing for $c>0$); we denote it as $cF(\nu)$. It means that a solution in $(-\frac{1}{2},\frac{1}{2})$ which corresponds to $\nu(\nu+1)\in(-\frac{1}{4},\frac{3}{4})$ exists iff $cF(\nu)\in(-1,1)$. On the other hand, for $\nu=-\frac{1}{2}+i\beta$ the eq.(3.6a) can be after simple manipulations rewritten in the form

$$\mathrm{ch}(\pi\beta)=-c\pi^2|\Gamma(\tfrac{3}{4}+i\beta)|^{-4} \quad . \tag{3.6b}$$

It is clearly sufficient to consider $\beta\geq 0$. The rhs (which we denote as $-cG(\beta)$) is increasing for $c<0$, but not so fast as $\mathrm{ch}(\pi\beta)$; its asymptotics for large β is $-\frac{1}{4}c\,e^{\pi\beta-3/2}\beta^{-1}[1+O(\beta^{-1})]$. Hence (3.6b) has a solution if $-cG(0)\geq 1$; one can check $\mathrm{ch}(\pi\beta)>G(\beta)/G(0)$ for all $\beta\neq 0$ so there is no solution if $-cG(0)<1$.

The above considerations allow us to calculate the sought critical values : we obtain

$$c_{nsa}=2\left(\frac{\Gamma(5/4)}{\Gamma(3/4)}\right)^2=1.09422\ldots \tag{3.7a}$$

and

$$c_{coll}=-2\left(\frac{\Gamma(3/4)}{\Gamma(1/4)}\right)^2=-\pi^{-2}\,\Gamma(3/4)^4=-0.22847\ldots \tag{3.7b}$$

4. The Admissible Hamiltonians

As mentioned in the introduction, our model consists of a free spinless particle moving in two halfspaces (with Neumann boundary conditions) which are connected at one point. The state Hilbert space of such a system is

$$\mathcal{H}=L^2(\mathbb{R}^2\times\mathbb{R}_+)\oplus L^2(\mathbb{R}^2\times\mathbb{R}_+) \quad . \tag{4.1}$$

Since the particle is assumed to be free anywhere except at the point singularity, a suitable starting operator for constructing the Hamiltonian is

$$H_0=H_{0,1}\oplus H_{0,2} \quad , \tag{4.2}$$

where $H_{0,j}=h_0$ for $j=1,2$. According to Proposition 2.2, the deficiency indices of H_0 are (2,2) so there is a four-parameter family of self-adjoint extensions H_U specified by 2×2 unitary matrices U . The decomposition (2.10) shows that each extension is of the form

$$H_U=A_U\oplus\bigoplus_{l=1}^{\infty}\overline{h_{0,1}^{(l)}\otimes I}\oplus\bigoplus_{l=1}^{\infty}\overline{h_{0,2}^{(l)}\otimes I} \quad , \tag{4.3}$$

where $h_{0,j}^{(l)}=h_0^{(l)}$ for $j=1,2$ (it makes no difference how we number the halfspaces) and A_U is some self-adjoint extension of the operator A_0 :

$$A_0=(h_{0,1}^{(0)}\otimes I)\oplus(h_{0,2}^{(0)}\otimes I) \tag{4.4a}$$

which acts on the Hilbert space

$$\mathcal{H}_0=(L^2(\mathbb{R}_+,r^2dr)\otimes\mathcal{K}_0)\oplus(L^2(\mathbb{R}_+,r^2dr)\otimes\mathcal{K}_0) \quad . \tag{4.4b}$$

Here $\mathcal{K}_0$ is the one dimensional subspace in $L^2(S_+^{(2)})$ spanned by the constant function f_{00} ; the angular part is therefore trivial and we shall drop it out in the following.

The adjoint operator A_0^* is given by the same differential expression as A_0 (cf.Ref.20, Appendix to Sec.X.1) so the deficiency subspaces $\mathcal{K}^{(\pm)}=\mathrm{Ker}(A_0^*\pm iI)$ can be found easily : they are spanned by the functions

$$\varphi_1^{(+)}=\begin{pmatrix}f_0\\0\end{pmatrix}\ ,\quad \varphi_2^{(+)}=\begin{pmatrix}0\\f_0\end{pmatrix}\ , \tag{4.5a}$$

where

$$f_0(r) = \frac{e^{-\bar{\varepsilon} r}}{r} \quad , \quad \varepsilon = e^{\pi i/4} \tag{4.5b}$$

and

$$\varphi_j^{(-)} = \overline{\varphi_j^{(+)}} \quad , \quad j = 1,2 \quad . \tag{4.5c}$$

According to the von Neumann theory, we have

$$A_U \subset A_0^* \tag{4.6a}$$

and every extension is specified by its domain,

$$D(A_U) \equiv D_U = \{ f = \varphi + c_1(\varphi_1^{(+)} + u_{11}\varphi_1^{(-)} + u_{12}\varphi_2^{(-)}) + \\ + c_2(\varphi_2^{(+)} + u_{21}\varphi_1^{(-)} + u_{22}\varphi_2^{(-)}) \ : \ c_1, c_2 \in \mathbb{C} \ , \varphi \in D(\bar{A}_0) \} \ , \tag{4.6b}$$

where u_{jk} are the matrix elements of U .

Not every extension is interesting, however. It is reasonable to suppose that the two halfspaces are physically equivalent, i.e., to require the extensions H_U to commute with the modified parity operator P which is defined on $\mathcal{H}$ by

$$P\begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \begin{pmatrix} \psi_2 \\ \psi_1 \end{pmatrix} \quad . \tag{4.7}$$

In the following, we restrict therefore our attention to such extensions A_U which fulfil

$$P_0 A_U \subset A_U P_0 \quad , \tag{4.8a}$$

where $P_0 = P \restriction \mathcal{H}_0$, or more explicitly, $P_0 D_U \subset D_U$ and $P_0 A_U = A_U P_0$ for $\psi \in D_U$. An inspection of the relations (4.6) shows that it is equivalent to

$$u_{11} = u_{22} \quad , \quad u_{12} = u_{21} \quad , \tag{4.8b}$$

since $P_0 \varphi_1^{(\pm)} = \varphi_2^{(\pm)}$ and $P_0 \bar{A}_0 \subset \bar{A}_0 P_0$. The family of extensions selected in this way is therefore two-parametric and its elements can be specified by the matrices

$$U = e^{i\xi} \begin{pmatrix} \cos\beta & i \sin\beta \\ i \sin\beta & \cos\beta \end{pmatrix} \tag{4.9}$$

with $\beta, \xi \in [0, 2\pi)$.

5. Characterization of the Extensions Through Boundary Conditions

According to (4.6a), every extension acts as the differential operator (2.9a) with $l=0$ on each component of the wave function. The expression (4.6b) of the domain D_U , however, is not very suitable for practical calculations ; one would prefer rather to have some boundary conditions in the connection point. Since the deficiency functions (4.5) are singular there, one must introduce regularized boundary values similarly as in Refs.4,16,17 :

$$L_0(f) = \lim_{r \to 0+} r f(r) \quad , \tag{5.1a}$$

$$L_1(f) = \lim_{r \to 0+} [f(r) - L_0(f) r^{-1}] \quad . \tag{5.1b}$$

Before proceeding further, we shall make one more restriction in the class of considered extensions. If the matrix U is diagonal, then one can see directly from (4.3) and (4.6b) together with the von Neumann formula for $A_U f$ that H_U is reduced by the projections E_j on the subspaces of $\mathcal{H}$ referring to the two halfspaces ; the situation is completely analogous to what happens for a diagonal U in the models treated in Refs.16,17 . In such a case, motion in the two parts of the configuration manifold is separated ; the particle cannot pass through the singularity to the other halfspace. Since this situation is not interesting from the viewpoint of modelling a thin-film contact, we restrict our attention in the following to the operators H_U corresponding to non-diagonal matrices U only.

5.1 Proposition : Each operator H_U which is not reduced by the projections E_j is of the form (4.3), where the operator $A_U \subset A_0^*$ is characterized uniquely by its domain specified by the following requirements :

(i) $f = \begin{pmatrix} f_1 \\ f_2 \end{pmatrix}$ with $f_j, f_j' \in AC[\mathbb{R}_+]$ and $h^{(0)} f_j \in L^2(\mathbb{R}_+, r^2 dr)$, $j = 1,2$,

(ii) the functions f_j fulfil the following boundary conditions at $r=0$:

$$L_0(f_1) = a L_0(f_2) + b L_1(f_2) \quad , \\ L_1(f_1) = c L_0(f_2) + d L_1(f_2) \quad , \tag{5.2}$$

where the coefficients a,b,c,d are related to the elements of a non-diagonal 2×2 unitary matrix U by

$$a = 2^{-1/2}\,\bar{\varepsilon}\,u_{12}^{-1}(i + iu_{11} - u_{22} - \det U) \quad , \tag{5.3a}$$

$$b = 2^{-1/2}\, i\, u_{12}^{-1}(1 + \mathrm{tr}\,U + \det U) \quad , \tag{5.3b}$$

$$c = 2^{-1/2}\, u_{12}^{-1}(-1 - i\,\mathrm{tr}\,U + \det U) \quad , \tag{5.3c}$$

$$d = 2^{-1/2}\,\bar{\varepsilon}\, u_{12}^{-1}(-i + u_{11} - iu_{22} + \det U) \quad . \tag{5.3d}$$

In particular, for the extensions commuting with the operator (4.7) we have

$$a = -d = \frac{\cos\beta + \cos\xi - \sin\xi}{\sin\beta} \quad , \tag{5.4a}$$

$$b = 2^{1/2}\,\frac{\cos\xi + \cos\beta}{\sin\beta} \quad , \tag{5.4b}$$

$$c = 2^{1/2}\,\frac{\sin\xi - \cos\beta}{\sin\beta} \quad , \tag{5.4c}$$

where the parameters $\beta \neq 0$ and ξ refer to the matrix (4.9).

Proof : Each $\varphi \in D(\bar{A}_0)$ fulfils the condition (i), and the same is true for any linear combination of the deficiency functions. In view of (4.6b) and (5.1), the condition (5.2) yield the following equations for the coefficients a,b,c,d :

$$\begin{aligned} 1 + u_{11} &= au_{12} - b\varepsilon u_{12} \quad , \\ u_{21} &= a(1 + u_{22}) - b(\bar{\varepsilon} + \varepsilon u_{22}) \quad , \\ -\bar{\varepsilon} - \varepsilon u_{11} &= cu_{12} - d\varepsilon u_{12} \quad , \\ -\varepsilon u_{21} &= c(1 + u_{22}) - d(\bar{\varepsilon} + \varepsilon u_{22}) \quad . \end{aligned} \tag{5.5}$$

Solving it, we obtain (5.3). and substituting from (4.9) for U , we arrive at the relations (5.4). It remains to check that the map $U \mapsto \{a,b,c,d\}$ is injective. Suppose that two matrices U,U′ lead to the same values of the coefficients. The relations (5.3) then give

$$\begin{aligned} i + iu'_{11} - u'_{22} - \det U' &= \alpha(i + iu_{11} - u_{22} - \det U) \quad , \\ 1 + \mathrm{tr}\,U' + \det U' &= \alpha(1 + \mathrm{tr}\,U + \det U) \quad , \\ -1 - i\,\mathrm{tr}\,U' + \det U' &= \alpha(-1 - i\,\mathrm{tr}\,U + \det U) \quad , \\ -i + u'_{11} - iu'_{22} + \det U' &= \alpha(-i + u_{11} - iu_{22} + \det U) \quad , \end{aligned} \tag{5.6}$$

where $\alpha = u'_{12}/u_{12}$; this number is non-zero by assumption. Taking suitable linear combinations of these relations, we get

$$u'_{11} - u'_{22} = \alpha(u_{11} - u_{22}) \quad , \tag{5.7a}$$

$$2^{1/2} + \varepsilon\,\mathrm{tr}\,U' = \alpha(2^{1/2} + \varepsilon\,\mathrm{tr}\,U) \quad , \tag{5.7b}$$

$$\varepsilon + \bar{\varepsilon}\det U' = \alpha(\varepsilon + \bar{\varepsilon}\det U) \quad , \tag{5.7c}$$

$$1 + u'_{11} = \alpha(1 + u_{11}) \quad . \tag{5.7d}$$

The first two of them give the relation $1 - i + 2u'_{11} = \alpha(1 - i + 2u'_{11})$, which is compatible with (5.7d) only if $\alpha = 1$. Hence we have $u'_{12} = u_{12}$, and using (5.7a,b) again, we get $u'_{jj} = u_{jj}$. Finally, combining these results with (5.7c), we obtain $u'_{21} = u_{21}$. ∎

6. The Transmission Coefficient

Let us now examine the situation when the particle passes from one half-space to the other one through the point singularity ; our aim is to find probability per unit time of the transmission. Similarly as in Refs.16-18, we use the time-independent approach, since it makes the problem more manageable. We start with the function $f = \begin{pmatrix} f_1 \\ f_2 \end{pmatrix}$, where

$$\begin{aligned} f_1(r) &= \frac{e^{-ikr}}{r} + A\,\frac{e^{ikr}}{r} \quad , \\ f_2(r) &= B\,\frac{e^{ikr}}{r} \quad , \end{aligned} \tag{6.1}$$

and demand it to belong locally to $D(A_U)$. Clearly $f_j, f'_j \in AC[\mathbb{R}_+]$ and $h^{(0)} f_j = k^2 f_j$ belongs to $L^2_{loc}(\mathbb{R}_+, r^2 dr)$. The boundary conditions (5.2) applied to (6.1) yield simple equations which are solved by

$$A(k) = \frac{ik(a+d) + c - bk^2}{ik(a-d) - c - bk^2} \tag{6.2a}$$

and

$$B(k) = \frac{2ik}{ik(a-d) - c - bk^2} \quad . \tag{6.2b}$$

We are interested in the extensions commuting with the operator (4.7), then the last relations reduce in the parametrization (4.9) to the form

$$A(k) = \frac{\sin\xi - \cos\beta - k^2(\cos\xi + \cos\beta)}{i\,2^{1/2}k(\cos\beta + \cos\xi - \sin\xi) - \sin\xi + \cos\beta - k^2(\cos\xi + \cos\beta)} \tag{6.3a}$$

$$B(k) = \frac{i\,2^{1/2} k \sin\beta}{i\,2^{1/2}k(\cos\beta + \cos\xi - \sin\xi) - \sin\xi + \cos\beta - k^2(\cos\xi + \cos\beta)} \;; \tag{6.3b}$$

it is easy to see that these coefficients fulfil

$$|A(k)|^2 + |B(k)|^2 = 1 \quad . \tag{6.4}$$

Let us ask now how the transmission coefficient can be derived from here. The S-matrix approach is not applicable, at least without a more sophisticated formulation, since we have no free Hamiltonian to compare. Instead, we shall calculate the probability current through the halfspheres of radius R in the two halfspaces. One obtains

$$j_1(R) = -\frac{\pi R^2}{2}\, 2\,\mathrm{Im}\left[\overline{f_1(r)}\,\frac{\partial f_1(r)}{\partial r}\right]_{r=R} = \pi k(1 - |A(k)|^2) \quad , \tag{6.5a}$$

where we set $\hbar = 2m = 1$ and the sign is chosen to correspond to the incoming probability current, and similarly

$$j_2(R) = \pi k |B(k)|^2 \quad . \tag{6.5b}$$

These quantities do not depend on R, so it is natural to interpret them as the probability current through the connection point. The transmission coefficient at the energy $E = k^2$ is therefore equal to

$$\mathcal{T}(E) = |B(k)|^2 = \tag{6.6}$$

$$= \frac{2k^2 \sin^2\beta}{2k^2(\cos\beta + \cos\xi - \sin\xi)^2 + (\sin\xi - \cos\beta + k^2(\cos\xi + \cos\beta))^2} \quad .$$

It is easy to see that there are two extensions (in the "parity preserving" class), namely those corresponding to $\xi = \frac{3}{4}$ and $\beta = \frac{\pi}{4}, \frac{7\pi}{4}$, which yield full transmission, $|A(k)|^2 = 1$. These are also the only cases in which the transmission coefficient is energy independent. Notice that the second named extension (with $\beta = \frac{7\pi}{4}$) corresponds to the situation when the wavefunctions are "glued together" in such a way that the regularized function $r \mapsto rf(r)$ is continuous at $r=0$ together with its first derivative.

7. The Case of Two Planes

In this section, we are going to discuss the second extreme case mentioned in the introduction, a free particle moving on two planes connected in one point. This situation has been analyzed in Ref.17, and our

aim here is to rephrase the results in a more suitable way. Recall that the boundary conditions can be written in terms of the regularized boundary values

$$L_0(f) = \lim_{r\to 0+} \frac{f(r)}{\ln r} \quad , \quad L_1(f) = \lim_{r\to 0+}\left[f(r) - L_0(f)\ln r\right] \quad . \tag{7.1}$$

The admissible Hamiltonians are of the form $H_U = A_U \oplus \tilde{h}$, where $\tilde{h}$ is a self-adjoint operator analogous to the second and third term in (4.3) (cf.Proposition 1 of Ref.17) and A_U is a self-adjoint operator on $L^2(\mathbb{R}_+, r\,dr) \oplus L^2(\mathbb{R}_+, r\,dr)$ which acts as

$$A_U\begin{pmatrix} f_1 \\ f_2 \end{pmatrix} = \begin{pmatrix} -\frac{1}{r}\frac{d}{dr}\left(r\,\frac{df_1}{dr}\right) \\ -\frac{1}{r}\frac{d}{dr}\left(r\,\frac{df_2}{dr}\right) \end{pmatrix} \quad . \tag{7.2}$$

The domain of A_U consists of the functions f with $f_j, f_j' \in AC[\mathbb{R}_+]$ and $A_U f_j \in L^2(\mathbb{R}_+, r\,dr)$, which are (for a given U) specified by suitable boundary conditions.

7.1 <u>Proposition</u> : The boundary conditions formulated in Proposition 3 of Ref.17 can be replaced for a non-diagonal U by

$$\begin{aligned} L_0(f_1) &= aL_0(f_2) + bL_1(f_2) \quad , \\ L_1(f_1) &= cL_0(f_2) + dL_1(f_2) \quad , \end{aligned} \tag{7.3}$$

where the coefficients a,b,c,d are related to the matrix elements of U as follows

$$a = u_{12}^{-1}[\chi(u_{11} - 1) + \bar{\chi}(\det U - u_{22})] \quad , \tag{7.4a}$$

$$b = \frac{2i}{\pi}\, u_{12}^{-1}[1 - \mathrm{tr}\, U + \det U] \quad , \tag{7.4b}$$

$$c = \frac{\pi i}{2}\, u_{12}^{-1}[\chi^2 + \bar{\chi}\chi\, \mathrm{tr}\, U + \bar{\chi}^2 \det U] \quad , \tag{7.4c}$$

$$d = u_{12}^{-1}[\chi(1 - u_{22}) + \bar{\chi}(u_{11} - \det U)] \quad , \tag{7.4d}$$

where $\chi \equiv L_1(f_0) = \frac{1}{2} + \frac{2i}{\pi}(\gamma - \ln 2)$ and $\gamma = 0.577216\ldots$ is the Euler's constant.

<u>Proof</u> can be performed in a complete analogy with that of Proposition 5.1 or of Proposition 3 of Ref.17 . Alternatively, one can write down and solve the linear relations between the boundary conditions (7.3) and those of Ref.17 . ■

Similarly as above, we are interested primarily in the extensions which commute with the modified parity operator which is defined on the state space of the present problem again by the relation (4.7). The admissible matrices U are then of the form (4.9) and the coefficients (7.4) can be rewritten as

$$a = -d = \frac{\sin\xi + \frac{4}{\pi}(\gamma - \ln 2)(\cos\beta - \cos\xi)}{\sin} , \quad (7.5a)$$

$$b = \frac{4}{\pi}\,\frac{\cos\xi - \cos\beta}{\sin\beta} , \quad (7.5b)$$

$$c = \frac{\pi}{2\sin\beta}\left[\frac{4}{\pi}(\gamma - \ln 2)\sin\xi + \left(\frac{1}{2} - \frac{8}{\pi^2}(\gamma - \ln 2)^2\right)(\cos\xi + \cos\beta)\right] \quad (7.5c)$$

Now we want to calculate the transmission coefficient. We start with $f = \binom{f_1}{f_2}$, where

$$f_1(r) = H_0^{(2)}(kr) + A(k)H_0^{(1)}(kr) , \quad (7.6a)$$

$$f_2(r) = B(k)H_0^{(1)}(kr) , \quad (7.6b)$$

and demand it to belong locally to $D(A_U)$. A simple calculation yields expressions for A,B which reduce in the "parity preserving" case to the form

$$A(k) = \frac{c - 2a(\gamma + \ln\frac{k}{2}) - b\left[\frac{\pi^2}{4} + (\gamma + \ln\frac{k}{2})^2\right]}{c - 2a(\frac{\pi}{2i} + \gamma + \ln\frac{k}{2}) - b(\frac{\pi}{2i} + \gamma + \ln\frac{k}{2})^2} , \quad (7.7a)$$

$$B(k) = \frac{-i\pi}{c - 2a(\frac{\pi}{2i} + \gamma + \ln\frac{k}{2}) - b(\frac{\pi}{2i} + \gamma + \ln\frac{k}{2})^2} ; \quad (7.7b)$$

it can be seen easily that they fulfil the relation (6.4). Then one can calculate the incoming (outgoing) probability current through the circle of radius R in the first (second) plane ; it holds

$$j_1(R) = 4(1 - |A(k)|^2) , \quad j_2(R) = 4|B(k)|^2 . \quad (7.8)$$

Notice that if we use instead the ansatz of Ref. 17, i.e., if the first term on the rhs of (7.6a) is replaced by $J_0(kr)$, then $j_1(R) = 1 - |1 + 2A(k)|^2 = 1 - |S_0(k)|^2$, where $S_0(k)$ is the s-wave scattering matrix. The relations (7.8) show that the transmission coefficient is equal to

$$\mathcal{T}(k^2) = |B(k)|^2 . \quad (7.9)$$

In distinction to the case of two halfspaces, no extension provides us with an energy-independent transmission coefficient. There is again one extension, namely the one corresponding to the matrix (4.9) with

$\xi = \beta = -\,\mathrm{arctg}\,(\frac{4}{\pi}(\gamma - \ln 2))$, such that the wavefunctions are joined "continuously" at r=0 as well as their "derivatives", but even in this case the transmission probability depends on energy :

$$\mathcal{T}(k^2) = \left[1 + \frac{4}{\pi^2}(\gamma + \ln\frac{k}{2})^2\right]^{-1} .$$

8. Conclusions

With the knowledge of the transmission coefficient $\mathcal{T}(E)$ as a function of energy, we are able to calculate the current-voltage characteristics. If the metals involved have the same Fermi energy, then the current is given by /24/

$$I = -\frac{2e}{\hbar}\int_0^\infty \mathcal{T}(E)\left[f_T(E) - f_T(E-eU)\right] dE , \quad (8.1a)$$

where e is the electron charge, U is the applied voltage, and

$$f_T(E) = \left[1 + \exp\left(\frac{E - E_F}{kT}\right)\right]^{-1} \quad (8.1b)$$

is the electron-gas density at the temperature T and Fermi energy E_F . The results are particularly simple in the zero-temperature limit. The differential resistance, e.g., is then given by

$$\frac{dU}{dI} = \frac{\hbar}{2e}\,\mathcal{T}(E_F + eU)^{-1} ; \quad (8.2)$$

this formula is of interest because dU/dI is a measured quantity, and the measurements are usually performed at temperatures of few K . To be just, we must mention that the formula (8.1) has been challenged, however, the alternative proposed in Ref.25 differs by an additive constant, which is unimportant for the argument presented below.

Let us turn now to the two extreme situations mentioned in the introduction. In the case when the "films" are very thick, which we can model by two halfspaces, we found two admissible Hamiltonians which yielded a transmission coefficient which is energy-independent, i.e., which gives a linear relation between the current and applied voltage. As we have remarked, the problem of choosing the right self-adjoint extension remains open. What is important, however, is that there are extensions leading to the Ohm's law in this simple model.

The situation is entirely different if the films are very thin. The analysis of Section 7 shows that the transmission coefficient is energy-dependent in this case for every extension. This is in contrast with the usual explanation[15] of the non-linear shape of current-voltage characteristics as a result of electron-phonon interaction. Our model shows that the Ohm's law should be expected to be violated for sufficiently thin films independently of any interaction.

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Экснер П., Шеба П. E5-86-693

Простая модель точечного контакта в тонких пленках в двух и трех измерениях

Рассматривается свободная бесспиновая квантовая частица, движущаяся на конфигурационном многообразии, состоящем из двух идентичных частей, соединенных в одной точке. Больше всего мы занимаемся трехразмерным случаем, когда этими частями являются полупространства с граничным условием Неймана; обсуждается коротко также случай более общего граничного условия. При помощи теории самосопряженных расширений построен класс допустимых гамильтонианов. Среди них особенный интерес проявляется к двухпараметрическому семейству, элементы которого инвариантны по отношению к замене полупространств; вычисляется коэффициент прохождения для каждого из этих расширений. Обсуждается также движение на двух плоскостях рассмотренное в нашей недавней работе; получена другая характеризация допустимых гамильтонианов. В заключение приведено сравнение этих двух случаев как моделей для экспериментов контактной спектроскопии в тонких пленках.

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Exner P., Šeba P. E5-86-693

A Simple Model of Thin-Film Point Contact in Two and Three Dimensions

We treat a free spinless quantum particle moving on a configuration manifold which consists of two identical parts connected in one point. Most attention is paid to the three-dimensional case when these parts are half-spaces with Neumann condition on the boundary; however, we discuss also briefly a more general boundary condition. The class of admissible Hamiltonians is constructed by means of the theory of self-adjoint extensions. Among them, a two-parameter family is particularly important whose elements are invariant with respect to exchange of the halfspaces; we compute the transmission coefficient for each of these extensions. We discuss also the motion on two planes considered in our recent paper, obtaining another characterization of the admissible Hamiltonians. In conclusions the two situations are compared as models for point-contact spectroscopical experiments in thin metallic films.

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

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