сообщения
объединенного
института
ядерных
исследований
дубна

E2-86-746

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MATHEMATICAL MODELS FOR QUANTUM POINT CONTACT SPECTROSCOPY

1986

1. Introduction

We sketch here two mathematical models intended to describe the point-contact spectroscopical experiments. It adds a new item to the list of recently discovered applications of the self-adjoint extensions theory.*)

The theory of self-adjoint extensions is a standard part of functional analysis for a more than half century. In the last years, it has attracted a new attention connected with interesting physical applications. Let us recall some of them:

(a) point interactions: one attempts to give a reasonable meaning to the formal Schroedinger operator

$$H = -\Delta + V(x) + \sum_{j=1}^{N} \lambda_j \delta(x-x_j) \qquad (1)$$

on $L^2(\mathbb{R}^d)$. A mathematically clean and effective way to performing this task starts with the operator $H_0 = -\Delta + V(x)$ defined on the domain from which the interaction points are removed,

$$D(H_0) = C_0^\infty(\mathbb{R}^d \setminus \{x_1,\dots,x_N\}) .$$

This operator is generally symmetric but not self-adjoint. One looks for its self-adjoint extensions which can be identified with the formal operator (1), with the coupling constants λ_j related to parameters of this extension.

There is a vast amount literature on this subject; let us mention, e.g. [1-5] . The method works for $d \leq 3$, since in higher dimensions removing of a point from the domain leaves the Schroedinger operator e.s.a. At present, the one-dimensional and three-dimensional cases are relatively well studied. The one-dimensional case has a more rich structure: if we restrict to one point interaction, then the deficiency indices are (1,1) for $d = 2,3$, and (2,2) for $d = 1$. Hence there are other self-adjoint extensions of H_0 for $d = 1$, e.g., the so-called δ'- interaction,

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*) A talk given on the 8th Congress of IAMP, Marseille, July,1986.

(b) another application, closely related to the previous one, concerns a one-dimensional model of three-particle collisions [6] in which impenetrable particles on a line interact via two-particle contact interactions plus three-particle contact interactions. Addition of the last term allows one to solve the model and determine resonance behaviour of the system,

(c) singular potentials: consider, e.g., a one-dimensional Schroedinger operator $H = -d^2/dx^2 + V(x)$ whose potential has a (repulsive) point singularity at $x = 0$; we ask whether tunnelling is possible between $\mathbb{R}^+$ and $\mathbb{R}^-$. It appears [7] that the answer is determined by the potential alone only if H is e.s.a.; the tunnelling is then forbidden if

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

for some $c > 0$. Otherwise the conditions (2) ensure absence of the tunnelling for the Friedrichs extension of H ; at the same time, a particle whose motion is governed by another extension of H can, in general, penetrate the barrier. This can be illustrated on the example of $V(x) = g\, x^{-2}$ with $0 < g < 3/4$, where the transmission coeficient may be calculated explicitly [7] for each 2x2 unitary matrix U characterizing a particular extension H_U ; it is zero iff U is diagonal. This result is interesting particularly from the viewpoint of conservation of topological charges in some field-theoretical models [8] ,

(d) again connected to the previous one, there is the problem of regularizing singular potentials. This is an often used trick to replace a Schroedinger operator with singular potential by a sequence of operators corresponding to suitably regularized potentials, and to study behaviour of its eigenvalues and other characteristics in the limit when the regularization is removed. If the original Schroedinger operator is not e.s.a., however, different regularisations may lead to different self-adjoint extensions [9,10] . Recall the example discussed in [9] : the operator

$$H_0^0 = -d^2/dx^2 + V(x)$$

with the natural domain

$$D(H_0^0) = D(-d^2/dx^2) \cap D(V)$$

for $V(x) = |x|^{-3/4} \chi_{[-1,1]}(x)$ is symmetric with the deficiency indices (1,1). Its self-adjoint extensions H_α can be constructed in a standard way; for the regularization procedure sketched on Fig. 1 one obtains

$$e^{i\alpha} = 1 + \frac{2\bar{\varepsilon}\, h}{h + 2\varepsilon} \int_{\mathbb{R}} |G(x,0,i)|^2 dx \tag{3}$$

depending on the parameter h, where $\varepsilon = e^{\pi i/4}$ and G is the Green's function of $H_0 = -d^2/dx^2 \dotplus V(x)$ (the form sum).

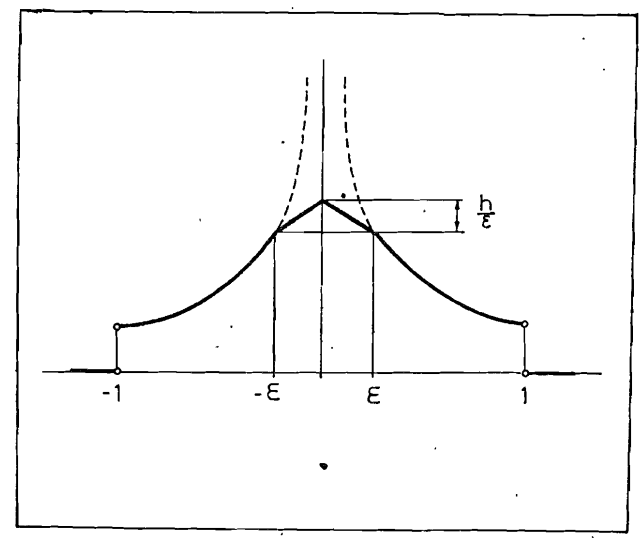


Fig.1. Scheme of a regularization procedure.

On the other hand, in the case of a stronger singularity, the sketched procedure leads to a single extension specified by Dirichlet boundary condition [11] .

(e) metallic model of a molecule, in which one starts with its graph (see Fig.2 for the anthracene molecule) and assigns to each of its links a suitable Schroedinger operator. The Hamiltonian is then obtained by "glueing" these operators together; it is nothing else than the choice of a self-adjoint extension. When combined with the free Hamiltonian in $\mathbb{R}^3$, this model can yield

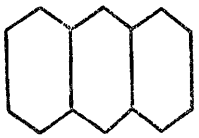


Fig.2. Graph of the anthracene molecule.

yield quasistationary states of the molecule as well [12,13] .

Let us stop the survey, though it is in no case complete. In what follows, we are going to demonstrate another possible application of the theory of self-adjoint extensions.

2. The quantum point-contact spectroscopy

For a metallic contact, the common wisdom suggests a linear relation between the applied voltage and the current according to the Ohm's law. This is true, if the size of the contact is large enough. On the other hand, once its diameter becomes comparable to the mean free path of electrons in the metal, interesting non-linear effects appear which gave rise to the new branch of research mentioned in the title; a review of this subject can be found in [14] . The small size of the contact causes scattering of the electrons giving a backward flow, which adds a negative and voltage-dependent contribution to the current.

Let us describe briefly typical experimental results illustrated on Figs. 3a,b and 4 adapted from [14] .

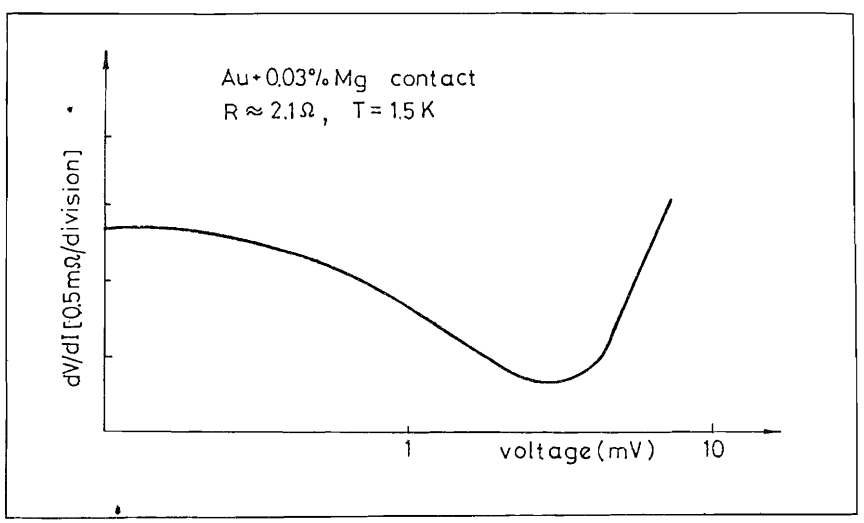
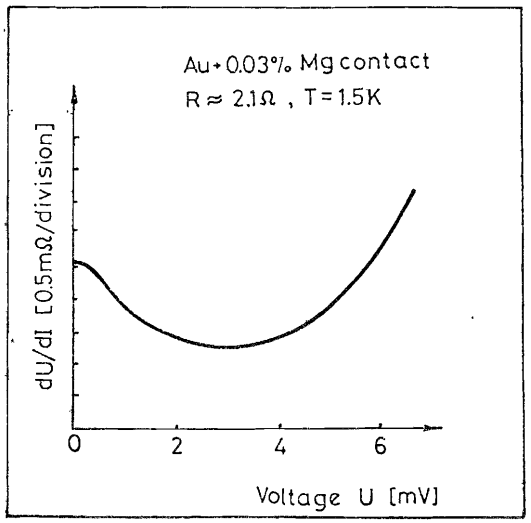


Fig. 3a. Measured differential resistance dV/dI for a point contact of the magnetically dilute alloy Au-0.03% Mn as a function of the applied voltage - logarithmic scale.

Fig.3b. Measured differential resistance for the Au-0.03% Mn contact as a function of the applied voltage - linear scale.



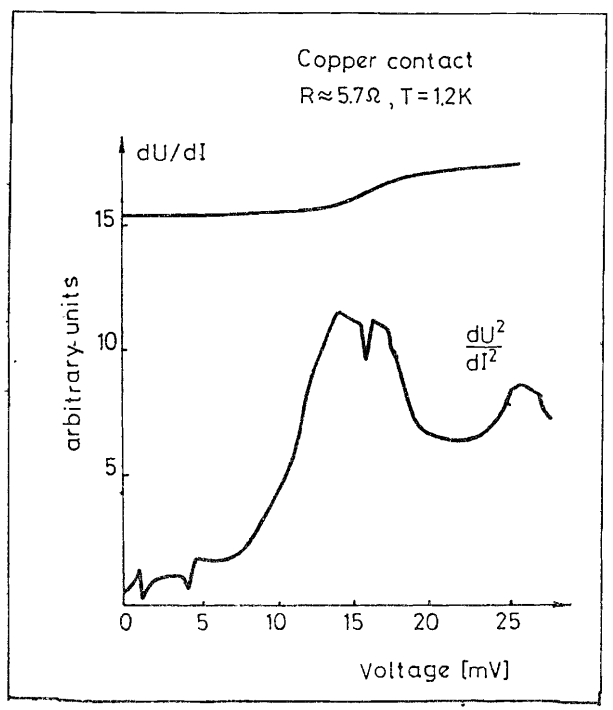


Fig.4. The current-voltage characteristics of a copper point contact.

The non-linear effects represent usually a few promile to a few percent of the total current. They are visible in the differential resistance dU/dI. The second derivative exhibits typically a more complicated shape with peaks corresponding to the metal involved; this is the most substantial information provided us by the method. Dependence of the characteristics on impurities in the metal, temperature, external magnetic field, etc., has been also studied

There are two types of point contacts. In the first of them, dubbed spear-and-anvil (or presure-type) contact, a sharply tipped wire is adjusted by a screw against a flat metallic surface. The second type consists of two thin metallic films separated by an insulating (oxide) layer which is perforated at one point. The contact diameter is typically a few Å . The device is placed into a suitable cooling medium, e.g., a liquid helium.

The theory of these contacts is certainly a complicated matter, and we are not going to discuss it here. Our aim is to show that simple mathematical models can be constructed which reproduce some features of such systems. To this purpose, we need an expression of the current. We restrict our attention to the case when the two parts of the contact are made of the same metal, or more generally, if they have the same Fermi energy. Then the current is given by [15]

$$I = -\frac{2e}{\hbar}\int_0^\infty T(E)\left[f_T(E) - f_T(E-eU)\right]\,dE, \qquad (4)$$

where e is the (positively taken) electron charge, U is the applied voltage, T(E) is the transmission coefficient, and

$$f_T(E) = \left(1 + \exp\left(\frac{E - E_F}{kT}\right)\right)^{-1} \qquad (5)$$

is the electron-gas density at the temperature T and Fermi energy E_F (the later is typically a few eV). The relation (4) becomes particularly simple in the zero temperature limit when

$$I = \frac{2e}{\hbar}\int_{E_F}^{E_F+eU} T(E)\,dE \quad ; \qquad (6)$$

evaluation of the differential resistance is straightforward in this case.

3. A model for the spear-and-anvil contact

The simplest model of this contact, in which its linear dimension is supposed to be zero, is represented by a free electron moving on the manifold consisting of a halfline connected to a plane (Fig.5). For simplicity we neglect spin of the electron so the state Hilbert space is $\mathcal{H} = L^2(\mathbb{R}^-) + L^2(\mathbb{R}^2)$. Such a system has been discussed in [16] ; we summarize here the results.

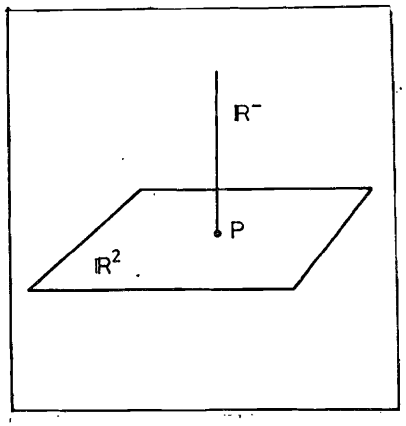


Fig.5. Configuration manifold for the model of spear-and-anvil contact.

Since the electron motion is supposed to be free except at the connection point, we start construction of Hamiltonian with the operator $H_0 = H_{0,1} \oplus H_{0,2}$, where

$$H_{0,1} = -d^2/dx^2$$
$$D(H_{0,1}) = C_0^\infty(\mathbb{R}^- \setminus \{0\}) \qquad (7a)$$
$$H_{0,2} = -\Delta$$
$$D(H_{0,2}) = C_0^\infty(\mathbb{R}^2 \setminus \{P\}) \quad . \qquad (7b)$$

The operator H_0 is not e.s.a. ; introducing polar coordinates in the plane, one finds easily that its deficiency indices are (2,2). Hence it possesses a four-parameter family of self-adjoint extensions, which can be constructed in a standard way; they are parametrized by 2x2 unitary matrices U.

It is useful to characterize the extensions by means of appropriate boundary conditions. In each pair of deficiency functions, one is singular at the connection point, but this difficulty can be bypassed by introducing the regularized boundary values [4]

$$L_0(\varphi) = \lim_{r\to 0}\frac{\varphi(r)}{\ln(r)}\ , \quad L_1(\varphi) = \lim_{r\to 0}\left[\varphi(r) - L_0(\varphi)\ln(r)\right]. \qquad (8)$$

For simplicity we restrict our attention to the case when

$$D(U) \equiv 1 + u_{11} - u_{22} - \det U \neq 0 \qquad (9).$$

(the remaining extensions are described in [16]). Then we have

Proposition 1: Under the condition (9), every extension H_U acts on $\varphi = \{\varphi_1, \varphi_2\} \in D(H_U)$ as

$$H_U\{\varphi_1,\varphi_2\} = \left\{-\frac{d^2}{dx^2}\varphi_1,\ -\Delta\varphi_2\right\},$$

and its domain $D(H_U)$ is a subspace in $D(H_0^*)$ specified uniquely by the following boundary conditions

$$\begin{aligned}\varphi_1'(0_-) &= A\,\varphi_1(0_-) + B\,L_0(\varphi_2)\\ L_1(\varphi_2) &= C\,\varphi_1(0_-) + D\,L_0(\varphi_2).\end{aligned} \tag{10}$$

The coefficients here are related to the matrix elements of U by

$$\begin{aligned}A &= \left[\bar{\varepsilon}(1-u_{22}) + \varepsilon(u_{11} - \det U)\right] D(U)^{-1}\\ B &= \pi 2^{-1/2}\,u_{21}\,D(U)^{-1}, \qquad C = u_{12}\,D(U)^{-1}\\ C &= \gamma - \ln 2 + \frac{\pi}{4i}\left[1 + \mathrm{tr}U + \det U\right]\cdot D(U)^{-1},\end{aligned} \tag{11}$$

where $\varepsilon = e^{\pi i/4}$ and $\gamma = 0.577216\ldots$ is the Euler's constant.

It is clear from the relations (10) and (11), that for a diagonal U, the boundary conditions separate; then H_U is of the form $H_{0,1}^{(A)} \oplus H_{0,2}^{(D)}$, the orthogonal sum of appropriate extensions of the operators (7). From the viewpoint of our model, this case is not interesting, since transmission between the two parts of the configuration manifold is impossible.

Assume therefore that U is non-diagonal. It is not difficult to calculate the reflection coefficient for an electron moving along the halfline; it equals to $|a_U(k)|^2$, where

$$a_U(k) = -\frac{(A-ik)\left[1+\frac{2i}{\pi}(\gamma - D + \ln\frac{k}{2})\right] + \frac{2i}{\pi}BC}{(A+ik)\left[1+\frac{2i}{\pi}(\gamma - D + \ln\frac{k}{2})\right] + \frac{2i}{\pi}BC}. \tag{12}$$

One can also consider scattering of an electron moving in the plane on the singular point. Only its s-wave part is non-trivial; the corresponding on-shell S-matrix is non-unitary and fulfils

$$1 - |S_0(k)|^2 = 1 - |a_U(k)|^2 .$$

In other words, the transmission probability is the same in both directions. This is just the quantity we need for evaluation of the current-voltage characteristics. In order to express it more explicitly, we parametrize the matrix U as follows

$$U = e^{i\varphi}\begin{pmatrix} e^{i(\alpha+\delta)}\cos\beta, & e^{i(\delta-\alpha)}\sin\beta \\ -e^{i(\alpha-\delta)}\sin\beta, & e^{-i(\alpha+\delta)}\cos\beta \end{pmatrix} \tag{13}$$

and introduce

$$\begin{aligned}\mathcal{S} &= \sin(\alpha+\delta+\tfrac{\pi}{4})\cos\beta - \sin(\varphi+\tfrac{\pi}{4}),\\ \mathcal{D} &= \sin(\alpha+\delta)\cos\beta - \sin\varphi,\\ \mathcal{C} &= \cos(\alpha+\delta)\cos\beta + \cos\varphi .\end{aligned}$$

Then one can calculate the transmission coefficient $T(k^2) = 1 - |a_U(k)|^2$ to be

$$T(k^2) = \frac{2^{1/2}\mathcal{D}^2\,k\sin^2\beta}{\mathcal{D}^2(\mathcal{S} - \frac{2}{\pi}\mathcal{D}k\ln k - \frac{1}{2}\mathcal{C}k)^2 + (\frac{1}{2}\mathcal{S}\mathcal{C} + \frac{2}{\pi}\mathcal{S}\mathcal{D}\ln k + \mathcal{D}^2 k + 2^{-3/2}\sin^2\beta)^2} \tag{14}$$

4. A model for the thin-film contact

We consider again the simplest possible model in which a free electron moves on the manifold consisting of two planes connected at one point (Fig.6), with neglection of the electron spin [17]. The state Hilbert space is therefore of the form $\mathcal{H} = L^2(\mathbb{R}^2) \oplus L^2(\mathbb{R}^2)$, and the construction starts from the operator $H_0 = H_{0,1} \oplus H_{0,2}$, where now both $H_{0,j}$ are given by (7b). The deficiency indices are again (2,2) so that there is a four-parameter family of self-adjoint extensions H_U of H_0 parametrized by 2x2 unitary matrices U. As in the preceding case, we restrict our attention to a class which contains most of them (referring to [17] for a complete description): we assume

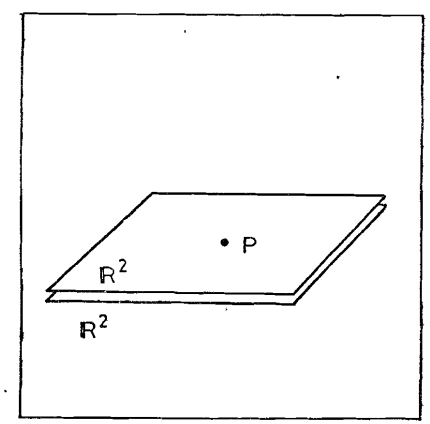


Fig.6. Configuration manifold for the model of thin-films contact.

$$D(U) \equiv 1 - \mathrm{tr}\,U + \det U \neq 0. \tag{15}$$

Then one has

Proposition 2: Under the condition (15), every extension H_U acts on $\varphi = \{\varphi_1, \varphi_2\} \in D(H_U)$ as $H_U \varphi = \{-\Delta\varphi_1, -\Delta\varphi_2\}$, and its domain $D(H_U)$ is a subspace in $D(H_0^*)$ determined by the boundary conditions

$$L_1(\varphi_1) = A\, L_0(\varphi_1) + B\, L_0(\varphi_2)\,,$$
$$L_1(\varphi_2) = C\, L_0(\varphi_1) + D\, L_0(\varphi_2)\,, \qquad (16)$$

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

$$A = \gamma - \ln 2 + \frac{\pi}{4i}\left[1 + u_{11} - u_{22} - \det U\right] D(U)^{-1}\,,$$
$$B = \frac{\pi}{2i}\, u_{21} D(U)^{-1}\,, \quad C = \frac{\pi}{2i}\, u_{12} D(U)^{-1}\,, \qquad (17)$$
$$D = \gamma - \ln 2 + \frac{\pi}{4i}\left[1 - u_{11} + u_{22} - \det U\right] D(U)^{-1}.$$

As in the preceding section, the case of a diagonal U is not interesting, because the motion is then separated between the two planes. Hence we assume again that U is non-diagonal, and consider scattering of an electron moving in the first plane on the singular point. For the s-wave, we get $S_0(k) = 1 + 2a_U(k)$, where

$$a_U(k) = \frac{\pi}{2iC}\left[1 + \frac{2i}{\pi}\left(\gamma - D + \ln\frac{k}{2}\right)\right] b_U(k) \qquad (18a)$$

and

$$b_U(k) = \frac{2i}{\pi}\, C\left\{\left[1 + \frac{2i}{\pi}\left(\gamma - A + \ln\frac{k}{2}\right)\right]\left[1 + \frac{2i}{\pi}\left(\gamma - D + \ln\frac{k}{2}\right)\right] + \frac{4}{\pi^2}BC\right\}^{-1} \qquad (18b)$$

while the remaining part of the S-matrix is trivial. The scattering is again non-unitary, and a straightforward calculation shows that $T(k^2) = 1 - |S_0(k)|^2$ equals

$$T(k^2) = 4\,|b_U(k)|^2\,, \qquad (19)$$

it is easy to check that this is the probability current through the connection point

5. Discussion

Using now the transmission coefficients (14) and (19), one can calculate the current-voltage characteristics. In particular, the differential resistance in the zero-temperature limit is

$$\frac{dU}{dI} = \frac{\pi}{2e}\, T(E_F + eU)^{-1}\,. \qquad (20)$$

The resulting function depends on the parameters specifying the self-adjoint extension used. Their choice requires an additional physical information; it schould be guided by some concept of what happens to an electron passing througt the contact. However, we are not going to discuss this question here.

We limit ourselves with illustrating how much the described method can reproduce the measured quantities. Consider the model of Section 3. The rhs of (20) has four adjustable parameters, with the help of which it is possible to fit the "background" non-linear shape of dU/dI just to give an example, we plot on Fig.7 the corresponding function for six extensions . The unpleasant feature of the model is that the resistance is growing at large U : it behaves like $\sim U^{1/2}(\ln U)^2$. Similar results can be obtained for the model of Section 4 - cf. Figs. 3a,b, 4,7,8 and 9.

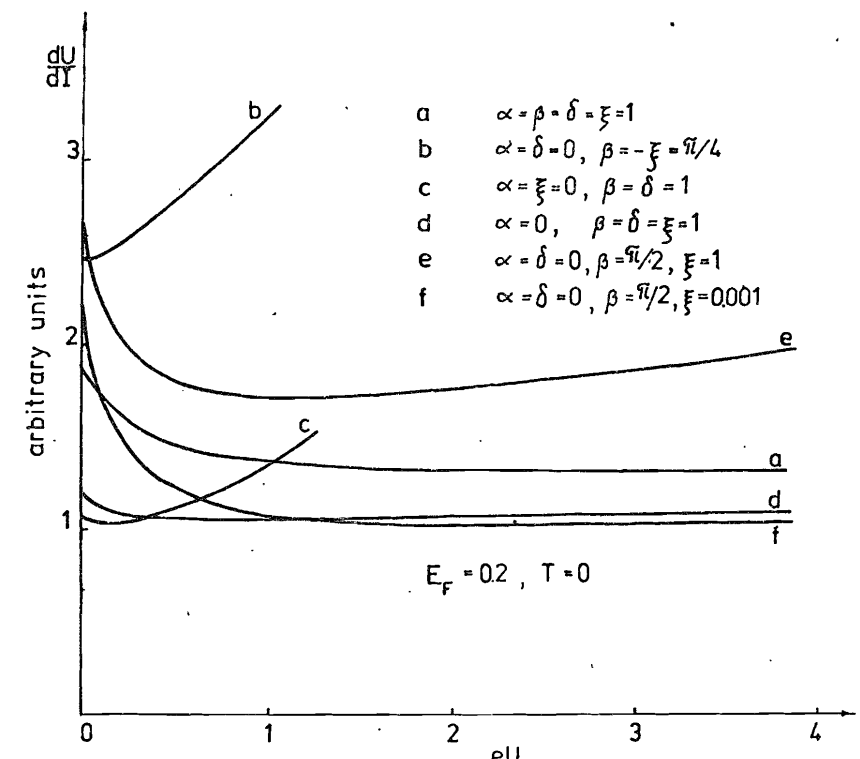


Fig. 7. Differential resistance for various self-adjoint extensions in the model of spear-and-anvil contact. The Fermi energy is taken to be $E_F = 0.2$.

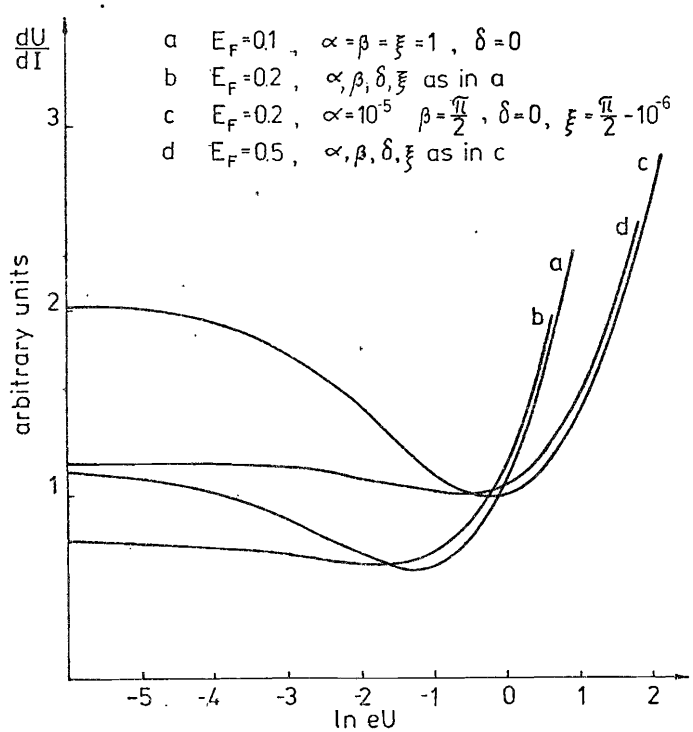


Fig. 8. Differential resistance for various self-adjoint extensions and various Fermi energies in the model of thin-films contact. The logarithmic scale.

On the other hand, the models under consideration cannot give a more complicated structure of the current-voltage characteristics, such as peaks in the second derivative, etc. This is, however, not surprising, because it reflects structure of the metal which has been completely neglected in our considerations, where the electrons are assumed to be free.

In conclusion, let us mention a preliminary results concerning another model of the pressure-type contact. In this model the plane is replaced by a half-space to which a halfline is attached. One must specify now how the electrons behave on the surface of such a "plane"; this is achieved by imposing the Neumann conditions on the boundary plane, with exclusion of the connection point.

Adding now a potential to the halfspace part of the "pre - Hamiltonian" and taking a particular extension, we obtain zero-

temperature resistance curves with a few peaks. According to our opinion, this is the line, along which models of this type should be developed further.

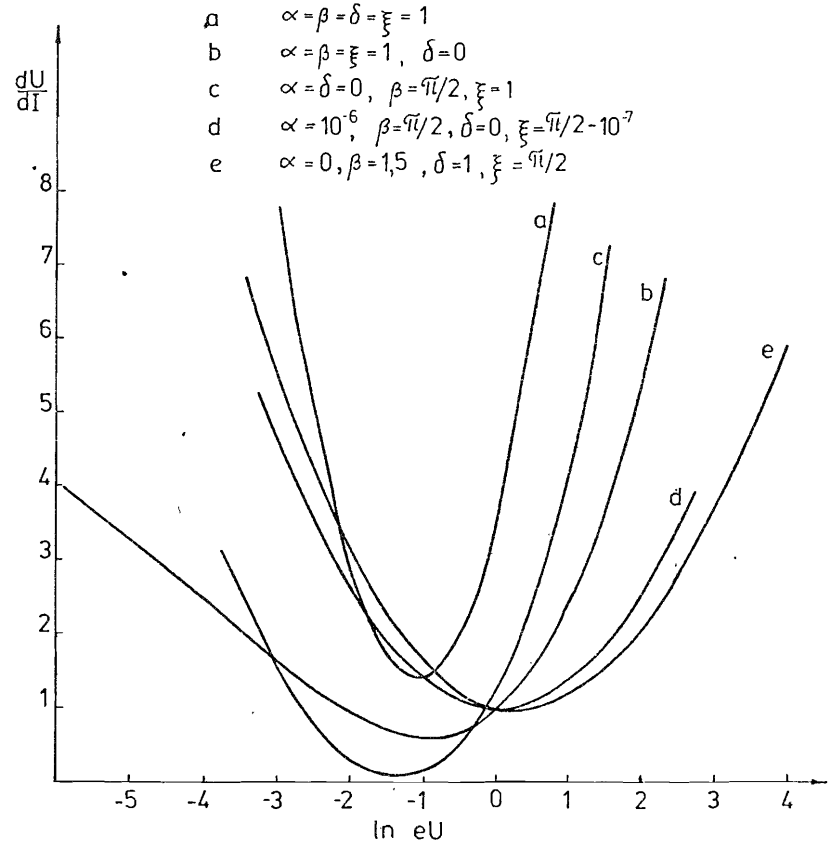


Fig. 9. Differential resistance for various self-adjoint extensions in the model of thin-films contact. The Fermi energy equals zero.

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Received by Publishing Department
on November 17, 1986.

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Экснер П., Шеба П. E2-86-746
Математические модели для квантовой контактной спектроскопии

Приводятся две простые математические модели, целью которых является описание экспериментов в квантовой контактной спектроскопии. Это добавляет еще одно название к списку недавно открытых применений теории самосопряженных расширений.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Сообщение Объединенного института ядерных исследований. Дубна 1986

Exner P., Šeba P. E2-86-746
Mathematical Models for Quantum Point Contact Spectroscopy

We sketch two mathematical models intended to describe the point contact spectroscopical experiments. It adds a new item to the list of recently discovered applications of the self-adjoint extension theory.

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

Communication of the Joint Institute for Nuclear Research. Dubna 1986