QUANTUM-MECHANICAL SPLITTERS: HOW SHOULD ONE UNDERSTAND THEM?

P. EXNER [1] and P. ŠEBA [2]
Laboratory of Theoretical Physics, JINR, 141980 Dubna, USSR

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To describe quantum oscillations on metallic rings and similar effects, some authors introduced recently an ideal device which "splits" the electron wavefunction at the junction of three "wires". A proper quantum-mechanical treatment requires, however, that the splitting procedure is described by a hamiltonian. In this Letter we show how this can be achieved in the framework of the self-adjoint-extension theory.

The behaviour of the conductivity for various systems of very thin metallic leads such as rings forming a loop on a lead, or the Cayley tree, has attracted recently a lot of attention [1–4]. For a description of such processes, the behaviour of the electron wavefunction at the branching point is crucial. In this Letter we are going to analyze this problem in the simplest case when the configuration manifold consists of three semi-infinite "wires".

Shapiro [1] suggested to associate an ideal device – a "splitter" – with a branching point which mediates the transmission of the entering electrons to the outgoing branches. The device is described by a matrix S which is momentum-independent and chosen in such a way that the incoming electron is never reflected back. A similar approach has been adopted in refs. [2,3,5], though the term "device" is not used explicitly there.

The role that the ideal device should play is not clear. Two possibilities arise: either it is a measuring instrument or it is an intrinsic part of the system. The first possibility is, however, excluded. According to the general principles of quantum mechanics [6], the state of an electron after passing such a device would be a mixture of states referring to the first and second outgoing lead. In that case, however, no interference is possible when we join the loose ends of the outgoing "wires", and this contradicts the experimental evidence [7].

The other possibility means that the electron motion is governed by a hamiltonian. Our goal is to show that such hamiltonians exist. We shall restrict ourselves to the simplest situation when the electron is supposed to be free everywhere except at the junction; modifications with addition of a potential interaction are straightforward as far as the potential remains bounded. The method of constructing the hamiltonians is based on the theory of self-adjoint extensions; it has been applied recently to another type of conductivity problem [8–10]. We shall explain the main idea; a more detailed exposition and proofs together with application to metallic rings will be given in a forthcoming paper.

Since we deal with three semi-infinite "wires", the state space is $L^2(\mathbb{R}^+)\oplus L^2(\mathbb{R}^+)\oplus L^2(\mathbb{R}^+)$. The construction of the hamiltonian starts from the operator

$$H_0 = \bigoplus_{j=1}^{3} H_{0,j}\,, \tag{1}$$

[1] On leave of absence from Nuclear Physics Institute, Czechoslovak Academy of Sciences, 250 68 Řež near Prague, Czechoslovakia.
[2] On leave of absence from Nuclear Centre, Charles University, V Holešovičkách 2, 180 00 Prague, Czechoslovakia.

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where each $H_{0,j}$ acts as $H_{0,j}f_j=-f_j''$ and its domain consists of all $f_j\in L^2(\mathbb{R}^+)$ with absolutely continuous derivatives and $f_j''\in L^2(\mathbb{R}^+)$ such that

$$0=f_j(0)=f_j'(0)\,,\quad j=1,2,3\,, \tag{2}$$

where the values at 0 are understood as the limits from the right. The operator H_0 is not self-adjoint; one must find therefore its self-adjoint extensions and choose the hamiltonian among them. The extensions are constructed in a standard way using von Neumann's theory [11]. In our particular case, H_0 as well as its adjoint are differential operators. Then any extension H_U acts as

$$H_U\{f_1,f_2,f_3\}=\{-f_1'',-f_2'',-f_3''\}\,; \tag{3}$$

various extensions are distinguished by their domains which are subspaces in $D(H_0^*)$ specified by suitable boundary conditions.

The deficiency indices of H_0 are (3, 3) so there is a nine-parameter family of its self-adjoint extensions. This set is very wide and we may try to restrict the freedom in the choice of hamiltonian by additional assumptions. One possibility is to require the wavefunction to be continuous at the junction, i.e.,

$$f_1(0)=f_2(0)=f_3(0)\equiv f(0)\,. \tag{4a}$$

In that case we are left with a one-parameter family of extensions specified by the boundary condition

$$f_1'(0)+f_2'(0)+f_3'(0)=Cf(0)\,, \tag{4b}$$

where C is a real number. In fact the continuity requirement is very strong. If we consider the case of n semi-infinite "wires" connected at one point, we have an n^2-parameter family of admissible hamiltonians, but the condition

$$f_1(0)=\ldots=f_n(0)\equiv f(0) \tag{5a}$$

selects among them just the one-parameter family obeying

$$f_1'(0)+\ldots+f_n'(0)=Cf(0)\,. \tag{5b}$$

We remark also that the requirement (5a) implies full symmetry with respect to interchanges of the "wires".

One can start therefore with a weaker assumption, namely that the wavefunction is continuous when passing from "wire" 1 to "wire" 2, but the junction to the third "wire" may be "tuned". This assumption seems reasonable if one takes into account the way, e.g., in which the rings with leads are fabricated [7]. In such a case, the starting condition (2) corresponding to fully disconnected "wires" should be replaced by

$$f_1(0)=f_2(0)=0\,,\quad f_1'(0)=-f_2'(0)\,,\quad f_3(0)=f_3'(0)=0\,, \tag{6}$$

in which the first two "wires" remain partially connected via the first derivative of the corresponding wavefunctions. The deficiency indices are now (2, 2) so there is a four-parameter family of self-adjoint extensions. It can be shown that they are specified by the boundary conditions

$$f_1(0)=f_2(0)\,, \tag{7a}$$

$$f_3(0)=Af_1(0)+B[f_1'(0)+f_2'(0)]\,, \tag{7b}$$

$$f_3'(0)=Cf_1(0)+D[f_1'(0)+f_2'(0)]\,, \tag{7c}$$

where A, B, C, D are complex numbers fulfilling

$$B\bar{C}-\bar{A}D=1\,,\quad \mathrm{Im}(\bar{A}C)=\mathrm{Im}(\bar{B}D)=0\,; \tag{8}$$

for $A=-D=1$ and $B=0$, we recover the conditions (4).

Let us turn to a scattering on the branching point. We set

$$f_j(x)=a_{j,\mathrm{in}}e^{-ikx}+a_{j,\mathrm{out}}e^{ikx}\,,\quad j=1,2,3 \tag{9}$$

and demand these wavefunctions to belong *locally* to the domain of a particular extension. It yields a system of linear equations that makes it possible to express the column vector of $a_{j,\mathrm{out}}$ by means of the column vector made of $a_{j,\mathrm{in}}$. After solving the system of equations, we get

$$\boldsymbol{a}_{\mathrm{out}}=S\boldsymbol{a}_{\mathrm{in}}\,, \tag{10a}$$

where

$$S=\frac{1}{C+ik(2D-A)+2k^2B}\begin{pmatrix} -C+ikA & 2ik(D-ikB) & -2ik \\ 2ik(D-ikB) & -C+ikA & -2ik \\ 2ik(AD-BC) & 2ik(AD-BC) & -C-ik(2D+A)+2k^2B \end{pmatrix}. \tag{10b}$$

Notice that condition (8) implies $|AD-BC|=1$.

The most important feature of this result is that the S matrix is in general momentum-dependent. Hence one must be concerned not only with the fraction of electrons in different channels, but also with the shape of the transmitted wavefunction. This is illustrated in fig. 1. In some cases, the S matrix is k-independent. Using the conditions (8), one finds easily that such matrices form a two-parameter family

$$S=\frac{1}{2+|A|^2}\begin{pmatrix} -|A|^2 & 2 & 2\bar{A} \\ 2 & -|A|^2 & 2\bar{A} \\ 2A & 2A & |A|^2-2 \end{pmatrix}, \tag{11a}$$

with A complex, $D=-\bar{A}^{-1}$ and $B=C=0$. These are just the matrices used in ref. [2], apart from the fact that the authors have imposed there the ad hoc assumption that S must be real. Notice that most of the fully symmetric solutions (4) do not fall in this class; the only exception is represented by the case $A=-D=-1$, $B=C=0$. As for the "reflectionless" matrices S considered by Shapiro [1] and others, there is a one-parameter family of them given by (11a) with

$$A=\sqrt{2}\,e^{i\omega}\,, \tag{11b}$$

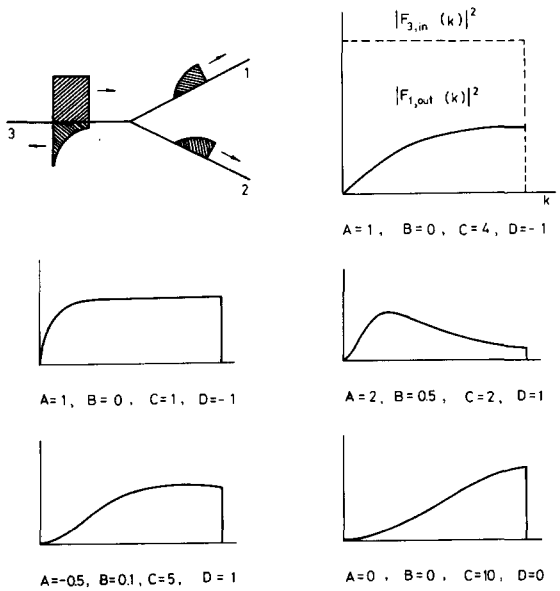

Fig. 1. The shape of the transmitted wavefunction for various matrices S. The incoming wave is rectangular.

where ω is a real number. None of the corresponding extensions is fully symmetric.

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