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FREE QUANTUM MOTION ON A BRANCHING GRAPH.
Construction of the Extensions

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1. Introduction

For many decades, the motion of a quantum particle on a line represented a useful abstraction and an introductory chapter to textbooks rather than a real problem. The situation changed during a last few years when the techniques became available which allowed to produce on a substrate thin metallic "wires" whose width was mere 250 Å .[1] By the same device, however, one can draw not only lines, but segments, circles,etc. as well. This opens a new frontier ; in order to give interpretation to the wide variety of conceivable experiments, one should build quantum mechanics on graphs and examine its implications.

At present, the experiment is clearly ahead of theory. A lot of conductivity measurements have been performed on the systems consisting of one or more metallic rings or similar structures[2-6]. A particular attention has been paid to the Aharonov-Bohm effect manifested by magnetoresistance oscillations. The size of involved graphs is so small that the phase destroying elastic scattering has a weak impact only ; in the nearest future, experiments with electrons in a purely ballistic regime are expected[6,7]. This is one reason why we shall discuss here the free motion. The other reason is that it represents the simplest possibility and a natural starting point for analysis of more complicated situations.

If we want to describe motion on a graph, it is crucial to know what happens at the branching points. In this paper, we are going to discuss this question for the simplest nontrivial graph that consists of three branches joined in one point. Since we have in mind mainly the electron motion in the metallic structures mentioned above, we refere to the branches as to wires in the following.

Shapiro[8] proposed to associate an ideal device called "splitter" with each branching point, however, he did not explain how it should be understood (see also Refs.9-11). Within the orthodox inter-

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pretation of quantum mechanics, two possibilities arise : either the splitter is a measuring device or a part of the system. The first possibility requires that we are able (at least, in principle) to determine which wire the electron has chosen after passing the junction. This is difficult, but conceivable. What is worse, state of the electron which went through such a device would be a mixture [12,13]. In such a case, however, the interference effects on the rings and similar structures will be impossible, and this contradicts to experimental evidence.

Hence the splitter must be a part of the system, and the time evolution of electrons passing through the junction must be described by a Hamiltonian. Then there is no necessity to introduce an extra device associated with the junction, because the information about the splitting process is contained fully in the Hamiltonian. The behaviour of a particular junction depends on the way in which it is fabricated, impurities of the material and other factors. They should be taken into account in a microscopic theory of such a contact. It is a difficult problem, however, and we are not going to discuss it here.

Instead, we shall discuss the abstracted situation in which the wires are supposed to be infinitely thin. In that case one can construct the class of all admissible Hamiltonians. Each of them is characterized by simple boundary conditions containing a few parameters. In turn, this makes it possible to calculate the matrix which describes scattering on the junction. It seems appropriate to us to reserve the term "splitter" for this matrix. The method of constructing the Hamiltonians is based on the theory of self-adjoint extensions*). We start with an operator which describes motion on the considered configuration manifold (three wires) with the connection point removed. Mathematically, the last statement is realized by choosing the initial domain as consisting of the functions which are zero on some neighbourhood of the junction. The operator obtained in this way is not essentially self-adjoint, and we shall construct its self-adjoint extensions. Similar ideas have been used recently within a different context in Refs.15-25.

Let us describe briefly the contents of the paper whose results have been announced in Ref.13. In the following section, we formulate the problem and construct the most general nine-parameter class of admissible Hamiltonians for the junction of three semiinfinite wires. We select here some important subclasses specified by the requirements of

*) The necessary information about the theory of self-adjoint extensions can be found in nearly all books on Hilbert-space operators - see, e.g., Ref.14 or Ref.27.

the wavefunction continuity or invariance with respect to permutations of the wires. They are discussed successively in Secs.3 and 5-8. In Sec.4, we present a generalization to the case of n wires. The second part of this paper [28] is devoted to calculation of the S-matrices, or splitters, for the Hamiltonians of the subclasses mentioned above. We shall discuss there also how the conclusions modify for wires of a finite length. Applications of the results derived here to analysis of the interference effects in metallic rings will be given in a subsequent paper.

2. Three semiinfinite wires

We shall be concerned mostly with the simplest nontrivial case when the configuration manifold consists of three halflines (Fig.1). The state Hilbert space of the problem is of the form

$$\mathcal{H} = L^2(\mathbb{R}^+) \oplus L^2(\mathbb{R}^+) \oplus L^2(\mathbb{R}^+) \quad . \tag{1}$$

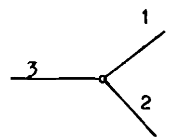

Fig.1 Connection of three semiinfinite wires.

Following the philosophy sketched in the introduction, we begin the construction of admissible Hamiltonians with the operator

$$H_0 = H_{0,1} \oplus H_{0,2} \oplus H_{0,3} \quad , \tag{2a}$$

where each $H_{0,j}$ acts as

$$H_{0,j} f_j = -f_j'' \tag{2b}$$

with the domain $D(H_{0,j}) = C_0^\infty(\mathbb{R}^+)$. Up to a certain degree, the choice of the domain is a matter of convenience ; one might take some larger one which is contained in $D(\overline{H}_{0,j}) = \{ f_j \in AC^2(\mathbb{R}^+) \, : \, f_j(0) = f_j'(0) = 0 \}$. Here $AC^2(\mathbb{R}^+)$ denotes conventionally the set of all $f_j \in L^2(\mathbb{R}^+)$ which are absolutely continuous together with their first derivatives and $f_j'' \in L^2(\mathbb{R}^+)$, furthermore, the values $f_j(0)$ and $f_j'(0)$ are understood as the limits from the right.

In order to see what can happen at the junction, one has to construct all self-adjoint extensions of the operator H_0 . Since each adjoint operator $H_{0,j}^*$ acts again according to the formula (2b) and its domain is $AC^2(\mathbb{R}^+)$, the deficiency subspaces are easily found : one has

$$\mathcal{K}_{\pm} \equiv \mathrm{Ker}(H_0^* \mp i) = \mathrm{lin}\{\varphi_1^{(\pm)}, \varphi_2^{(\pm)}, \varphi_3^{(\pm)}\} \quad , \tag{3}$$

where

$$\varphi_1^{(+)} = \{f_+, 0, 0\} \tag{4a}$$

and similarly for $j = 2,3$,

$$f_+(x) = e^{-\bar{\varepsilon} x} \tag{4b}$$

with $\varepsilon = e^{\pi i/4}$ and

$$\varphi_j^{(-)} = \overline{\varphi_j^{(+)}} \quad , \quad j = 1,2,3 \quad . \tag{4c}$$

Consequently, the deficiency indices of H_0 are $(3,3)$ and one has a nine-parameter family of self-adjoint extensions. Since the $\varphi_j^{(\pm)}$ are of the same norm, one can characterize the extensions by 3×3 unitary matrices U . Each extension H_U represents a restriction of H_0^* , i.e.,

$$H_U\{f_1, f_2, f_3\} = \{-f_1'', -f_2'', -f_3''\} \quad , \tag{5a}$$

and it is specified by its domain

$$D(H_U) = \left\{ f = \varphi + \sum_{j=1}^{3} c_j \left(\varphi_j^{(+)} + \sum_{k=1}^{3} u_{jk} \varphi_k^{(-)} \right) \; : \; c_j \in \mathbb{C} \; , \; \varphi \in D(\bar{H}_0) \right\}. \tag{5b}$$

The relations (5) represent a complete solution to our problem in terms of the von Neumann theory[14,27]. From the viewpoint of practical applications, however, the specification of the domain by means of the matrix U is not very suitable. Fortunately, one is able to classify the extensions alternatively by boundary conditions ; it will be done in the following sections.

Before proceeding further, let us mention some restrictions which might be imposed on the set of all extensions H_U . The latter represents a nine-parameter family, being therefore a bit too wide. Some interesting subfamilies are the following :

(a) the extensions that require the wavefunction to be continuous at the junction,

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

(b) a wider class than the preceding one : the extensions that require the wavefunction to be continuous when passing from wire 1 to wire 2 ,

$$f_1(0) = f_2(0) \quad ; \tag{7}$$

(c) the extensions invariant under permutations of the wires.

3. The extensions with continuous wavefunctions

In this section, we are going to discuss the first one of the above named classes of extensions. Let us substitute for f from (5b) to the continuity condition (6). Since the equality must hold for all complex c_j , we get

$$\begin{aligned} 1 + u_{11} &= u_{12} = u_{13} \quad , \\ 1 + u_{22} &= u_{21} = u_{23} \quad , \\ 1 + u_{33} &= u_{31} = u_{32} \quad . \end{aligned} \tag{8}$$

Hence the matrix elements of U can be expressed by means of u_{13}, u_{23} and u_{33} . The unitarity conditions then read

$$3|u_{j3}|^2 - 2\,\mathrm{Re}\, u_{j3} = 0 \quad , \quad j = 1,2 \quad , \tag{9a}$$

$$3|u_{33}|^2 + 4\,\mathrm{Re}\, u_{33} + 1 = 0 \quad , \tag{9b}$$

$$3\, u_{13}\bar{u}_{23} - u_{13} - \bar{u}_{23} = 0 \quad , \tag{9c}$$

$$3\, u_{j3}\bar{u}_{33} + 2\, u_{j3} - \bar{u}_{33} - 1 = 0 \quad , \quad j = 1,2 \quad . \tag{9d}$$

Subtracting the last two of them, and taking into account that $3\bar{u}_{33} + 2 \neq 0$ in view of (9b), we get $u_{13} = u_{23}$. Then it is sufficient to consider $j = 1$ only in (9a),(9d) , while (9c) is equivalent to (9a). Of the remaining three conditions, one is still superfluous : if we express u_{33} from (9d),

$$u_{33} = - \frac{1 - 2\bar{u}_{13}}{1 - 3\bar{u}_{13}} \quad , \tag{10a}$$

and substitute it to (9b), we arrive after a short calculation to (9a). The last named condition is solved by

$$u_{13} = \frac{2}{3}\, e^{i\beta} \cos\beta \quad , \quad \beta \in [0,\pi) \quad ; \tag{11a}$$

substituting it back to (10a), we obtain

$$u_{33} = u_{13} - 1 \quad . \tag{10b}$$

Summing the above argument, we see that there is a one-parameter family of extensions H_U with continuous wavefunctions, which correspond to matrices of the form

$$U = \begin{pmatrix} u_{13}-1 & u_{13} & u_{13} \\ u_{13} & u_{13}-1 & u_{13} \\ u_{13} & u_{13} & u_{13}-1 \end{pmatrix} \quad , \tag{11b}$$

where u_{13} is given by (11a). This matrix has a particular symmetry ; it means, as we shall demonstrate below, that the extensions with continuous wavefunctions are permutation-invariant.

Now we would like to characterize the extensions under consideration by suitable boundary conditions. Since the deficiency indices are (3,3) , the extensions are specified by three linearly independent conditions[26,27]. We try the condition

$$f_1'(0) + f_2'(0) + f_3'(0) = C f(0) \quad , \tag{12}$$

where $f(0)$ denotes the common boundary value of the functions f_j . Substituting from (5b) for f and using (11b), we get the relation $-\bar{\varepsilon} - \varepsilon(3u_{13} - 1) = C u_{13}$. In combination with (11a), it yields

$$C = -3\,\frac{\cos(\beta + \frac{\pi}{4})}{\cos\beta} \quad . \tag{13}$$

Hence the extensions with continuous wavefunctions are characterized by the boundary conditions (6) and (12) with a real number C . We include conventionally the possibility $C = \infty$ that corresponds to the boundary conditions $f_1(0) = f_2(0) = f_3(0) = 0$. It is easy to see that the correspondence $C \leftrightarrow U$ is one-to-one so the conditions (6) and (12) characterize uniquely all extensions of the class (a). The derivatives on the lhs of (12) cannot enter with different coefficients; it is one more manifestation of the fact that the extensions under consideration are permutation-invariant.

4. A diggression : the case of n wires

We have seen that the continuity requirement (6) reduces substantially the number of free parameters. In order to illustrate, how strong this requirement is, let us discuss the analogous situation for n semiinfinite wires (Fig.2). The relations (1)-(5) are easily adapted to this case. The operator H_0 has now deficiency indices (n,n) so it has a n^2-parameter family of self-adjoint extensions. Each of them is specified by (5b) with 3 replaced by n . Let us demand now the wavefunctions to be continuous at the junction, i.e., to fulfil

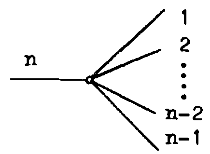

Fig.2 Connection of n semiinfinite wires

$$f_1(0) = \cdots = f_n(0) \quad . \tag{14}$$

It yields the relations

$$u_{j1} = \cdots = u_{j,j-1} = u_{jj} + 1 = u_{j,j+1} = \cdots = u_{jn} \tag{15}$$

for $j = 1,\dots,n$, which makes it possible to express the matrix elements of U by means of $u_{1n},\dots,u_{nn}$. The unitarity conditions then read

$$n|u_{jn}|^2 - 2\,\mathrm{Re}\,u_{jn} = 0 \quad , \quad j = 1,\dots,n-1 \quad , \tag{16a}$$

$$n|u_{nn}|^2 + 2(n-1)\mathrm{Re}\,u_{nn} + n - 2 = 0 \quad , \tag{16b}$$

$$n\,u_{jn}\bar{u}_{kn} - u_{jn} - \bar{u}_{kn} = 0 \quad , \quad j,k = 1,\dots,n-1 \quad , \tag{16c}$$

$$n\,u_{jn}\bar{u}_{nn} + (n-1)u_{jn} - \bar{u}_{nn} - 1 = 0 \quad , \quad j = 1,\dots,n-1 \quad . \tag{16d}$$

Now one has to subtract the conditions (16d) for different j,k ; since $n\bar{u}_{nn} + n - 1 = 0$ contradicts to (16b), we get $u_{jn} = u_{kn}$ for $j,k = 1,\dots,n-1$. Next one may use (16d) to express

$$u_{nn} = -\,\frac{1 - (n-1)\bar{u}_{1n}}{1 - n\bar{u}_{1n}} \quad . \tag{17a}$$

The condition (16b) then reduces to (16a) as well as (16c) ; we are left therefore with the condition (16a) for $j = 1$ alone. It is solved by

$$u_{1n} = \frac{2}{n} e^{i\beta} \cos\beta \quad , \quad \beta \in [0,\pi) \quad ; \tag{18a}$$

substituting it back to (17a), we get

$$u_{nn} = u_{1n} - 1 \quad . \tag{17b}$$

Hence the extensions that obey (14) are characterized by the matrices

$$U = \frac{2}{n} e^{i\beta} \begin{pmatrix} \cos\beta - \frac{n}{2} e^{-i\beta} & \cos\beta & \cdots & \cos\beta \\ \cos\beta & \cos\beta - \frac{n}{2} e^{-i\beta} & \cdots & \cos\beta \\ \cdots & \cdots & \cdots & \cdots \\ \cos\beta & \cos\beta & \cdots & \cos\beta - \frac{n}{2} e^{-i\beta} \end{pmatrix} \tag{18b}$$

with $\beta \in [0,\pi)$. We see that the continuity requirement selects just one-parameter family of extensions out of the n^2-parameter one. These extensions can be again characterized by boundary conditions. We set

$$f_1'(0) + \cdots + f_n'(0) = Cf(0) \quad , \tag{19}$$

where $f(0)$ is the common value of $f_j(0)$. It yields the conditions $-\bar{\varepsilon} - \varepsilon(u_{j1} + \cdots + u_{jn}) = Cu_{jn}$ for $j = 1,\ldots,n-1$ and $-\bar{\varepsilon} - \varepsilon(u_{n1} + \cdots + u_{nn}) = Cu_{n1}$, but in view of (18b), all of them reduce to a single condition which is solved by

$$C = -n \frac{\cos(\beta + \frac{\pi}{4})}{\cos\beta} \quad . \tag{20}$$

The corespondence $C \leftrightarrow U$ is again one-to-one, i.e., each extension H_U with continuous wavefunctions is characterized uniquely by the boundary conditions (14) and (19) with a real number C .

5. Three wires : another approach

Before examining the class (b) of Section 2, let us construct the extensions with continuous wavefunctions in another way. We are motivated by the fact that dealing with 3×3 matrices is not so simple, and that it is worth to formulate the problem in terms of 2×2 matrices when it is possible. We shall build now the junction successively, first joining the wires 1 and 2 , and afterwards attaching the third one to them (Fig.3).

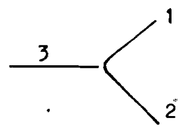

Fig.3 Successive joining of three wires

The first two wires together form a line. The free motion on it is described by the Hamiltonian which corresponds to $C = 0$, or $\beta = \pi/4$, and $n = 2$ in the relations (18)-(20). In order to join the third wire to the first two ones, it is necessary to "disconnect" them partially by setting $f_j(0) = 0$ for $j = 1,2$. The starting operator will therefore be $\tilde{H}_0 = H_{0,1+2} \oplus H_{0,3}$, where $H_{0,1+2}$ is the restriction of $H_{U(\pi/4)}$, the free Hamiltonian on the line, to

$$D(H_{0,1+2}) = \left\{ f = \{f_1,f_2\} \;:\; f_j \in AC^2(\mathbb{R}^+) \;,\; f_1(0) = f_2(0) = 0 \;,\; f_1'(0) = -f_2'(0) \right\} . \tag{21a}$$

The deficiency indices of the operator H_0 are $(2,2)$, and the deficiency subspaces are spanned by the vectors $\varphi_3^{(\pm)}$ defined in Sec.2 and by $\varphi_0^{(\pm)}$ given by

$$\varphi_0^{(\pm)} = 2^{-1/2}\{f_+,f_+,0\} \tag{22a}$$

with f_+ given by (4b) and

$$\varphi_0^{(-)} = \overline{\varphi_0^{(+)}} \quad . \tag{22b}$$

In order to check this assertion, one has to realize, that the wires 1 and 2 are now only partially disconnected, since the derivatives at 0 are allowed to be non-zero (and mutually correlated) within $D(H_{0,1+2})$. An easy integration by parts shows that the boundary conditions in (21a) yield

$$D(H^*_{0,1+2}) = \left\{ f = \{f_1,f_2\} \;:\; f_j \in AC^2(\mathbb{R}^+) \;,\; f_1(0) = f_2(0) \right\} . \tag{21b}$$

Hence the solutions to the deficiency equations must be joined continuously at 0 . In turn, it implies that the wavefunctions in the domain of any extension $\tilde{H}_U$ of $\tilde{H}_0$ are continuous when passing from wire 1 to wire 2 , because

$$D(\tilde{H}_{\tilde{U}}) = \left\{ f = \varphi + \sum_{j=0,3} c_j \Big(\varphi_j^{(+)} + \sum_{k=0,3} \tilde{u}_{jk} \varphi_k^{(-)} \Big) \;:\; c_j \in \mathbb{C} \;,\; \varphi \in D(\bar{\tilde{H}}_0) \right\} , \tag{23a}$$

where $\tilde{U}$ is a 2×2 unitary matrix whose rows and columns are indexed by 0 and 3 , and

$$D(\tilde{\bar{H}}_0) = \{ f = \{f_0, f_3\} :\ f_0 \in D(H_{0,1+2})\ ,\ f_3 \in D(\bar{H}_{0,3}) \} \ . \tag{23b}$$

Mimicking now the argument given in Sec.3, one can show easily that imposing additionaly the continuity requirement on the joint of the third wire, we arrive back at the one-parameter family of extensions characterized by the boundary conditions (6) and (12).

6. The extensions with partially continuous wavefunctions

The extensions of the class (b) are therefore fully described by the relations (5a) and (23a). Now we want to characterize them by suitable boundary conditions. We choose them in the form

$$f_1(0) = f_2(0) \ , \tag{24a}$$

$$f_3(0) = Af_1(0) + B(f_1'(0) + f_2'(0)) \ , \tag{24b}$$

$$f_3'(0) = Cf_1(0) + D(f_1'(0) + f_2'(0)) \ , \tag{24c}$$

where the first condition represents the requirement (7). Substituting from (23a), we get the following set of equations

$$\left.\begin{aligned} 2^{1/2}u_{03} &= A(1+u_{00}) - 2B(\bar{\varepsilon} + \varepsilon u_{00}) \ , \\ 2^{1/2}(1+u_{33}) &= Au_{30} - 2B\varepsilon u_{30} \ , \\ -2^{1/2}\varepsilon u_{30} &= C(1+u_{00}) - 2D(\bar{\varepsilon} + \varepsilon u_{00}) \ , \\ -2^{1/2}(\bar{\varepsilon} + \varepsilon u_{33}) &= Cu_{30} - 2D\varepsilon u_{30} \ , \end{aligned}\right. \tag{25}$$

which is solved by

$$A = \varepsilon u_{30}^{-1}(1 + iu_{00} + u_{33} + i\det U) \ , \tag{26a}$$

$$B = \frac{1}{2}\, u_{30}^{-1}(1 + \mathrm{tr}\, U + \det U) \ , \tag{26b}$$

$$C = -u_{30}^{-1}(1 + i\,\mathrm{tr}\, U - \det U) \ , \tag{26c}$$

$$D = -\frac{\varepsilon}{2}\, u_{30}^{-1}(1 + u_{00} + iu_{33} + i\det U) \tag{26d}$$

if only $u_{30} \neq 0$. The remaining extensions must be characterized in a different way, but it can be easily done. If $u_{30} = 0$, the matrix U is diagonal and the two parts of the configuration manifold remain separated as it can be seen from (23a). The Hamiltonian is then of the

form $\tilde{H}_U = H_{12} \oplus H_3$, where H_{12} describes motion on the line with a δ-interaction situated at 0 (cf. Refs.16,19), while H_3 is one of the standard free halfline Hamiltonians - cf.Ref.14, appendix to Sec. X.1 .

The complex coefficients A,B,C,D in (24) should parametrize the family of extensions given by (23a) with a non-diagonal U , and therefore they cannot be fully independent. We shall show that they obey the conditions

$$B\bar{C} - \bar{A}D = 1 \ , \tag{27a}$$

$$\mathrm{Im}(\bar{A}C) = \mathrm{Im}(\bar{B}D) = 0 \ , \tag{27b}$$

which leave just four real parameters free. The easiest way to check the relations (27) is to use an explicit parametrization of the matrix U , e.g.,

$$U = e^{i\xi} \begin{pmatrix} e^{i(\alpha+\delta)}\cos\beta & e^{i(\delta-\alpha)}\sin\beta \\ -e^{i(\alpha-\delta)}\sin\beta & e^{-i(\alpha+\delta)}\cos\beta \end{pmatrix} . \tag{28}$$

Substituting it to (26), we get

$$A = -2i\, e^{i(\delta-\alpha)} \left[\cos(\alpha + \delta + \tfrac{\pi}{4})\cos\beta + \cos(\xi + \tfrac{\pi}{4})\right](\sin\beta)^{-1} \ , \tag{29a}$$

$$B = -i\, e^{i(\delta-\alpha)} \left[\cos(\alpha+\delta)\cos\beta + \cos\xi\right](\sin\beta)^{-1} \ , \tag{29b}$$

$$C = 2i\, e^{i(\delta-\alpha)} \left[\cos(\alpha+\delta)\cos\beta - \sin\xi\right](\sin\beta)^{-1} \ , \tag{29c}$$

$$D = i\, e^{i(\delta-\alpha)} \left[\cos(\alpha + \delta - \tfrac{\pi}{4})\cos\beta + \cos(\xi + \tfrac{\pi}{4})\right](\sin\beta)^{-1} \ . \tag{29d}$$

It is evident now that (27b) is valid, (27a) follows from (29) after a short calculation. Moreover, the conditions (27) imply also

$$\mathrm{Im}(\bar{A}B) = \mathrm{Im}(\bar{A}D) = \mathrm{Im}(\bar{B}C) = \mathrm{Im}(\bar{C}D) = 0 \ , \tag{30a}$$

$$|AD - BC| = 1 \ . \tag{30b}$$

Next one has to check that the correspondence $U \leftrightarrow \{A,B,C,D\}$ is bijective. It can be verified directly that for A,B,C,D which obey (27), the equations (29) have a solution. Suppose further that the matrices U, U' yield the same values of the coefficients. In view of (26), we have

$$1+iu'_{00}+u'_{33}+i\det U' = \alpha(1+iu_{00}+u_{33}+i\det U)\,, \tag{31a}$$

$$1+\mathrm{tr}\,U'+\det U' = \alpha(1+\mathrm{tr}\,U+\det U)\,, \tag{31b}$$

$$1+i\,\mathrm{tr}\,U'-\det U' = \alpha(1+i\,\mathrm{tr}\,U-\det U)\,, \tag{31c}$$

$$1+u'_{00}+iu'_{33}+i\det U' = \alpha(1+u_{00}+iu_{33}+i\det U)\,, \tag{31d}$$

where $\alpha = u'_{30}/u_{30}$. Summing (31b) and (31d), and subtracting (31d) from (31a), we get the relations

$$\sqrt{2}+\varepsilon\,\mathrm{tr}\,U' = \alpha(\sqrt{2}+\varepsilon\,\mathrm{tr}\,U)$$

and

$$\varepsilon(u'_{33}-u'_{00}) = \alpha\varepsilon(u_{33}-u_{00}) \tag{32a}$$

which together yield

$$1-i+u'_{33} = \alpha(1-i+u_{33})\,. \tag{32b}$$

Subtracting the last relation from (31a), we get $1+u'_{00}+\det U' = \alpha(1+u_{00}+\det U)$. In combination with (31b), it gives $u'_{33}=\alpha u_{33}$ so $\alpha=1$ follows from (32b). Then $u'_{00}=u_{00}$ due to (32a) and $\mathrm{tr}\,U'=\mathrm{tr}\,U$. Furthermore, the definition of α implies $u'_{30}=u_{30}$. Since $\det U'=\det U$ holds in view of (31b), we get $u'_{03}u_{30}=u_{03}u_{30}$. However, $u_{30}\neq 0$ by assumption, and therefore $U'=U$.

7. The permutation-invariant extensions

Let us turn now to the last subclass mentioned in Sec.2 that contains the extensions which are invariant under permutations of the wires. In other words, we require now the wires to be physically equivalent. The operators P_{jk} representing transposition of a pair of wires act in the following simple way

$$P_{12}\{f_1,f_2,f_3\} = \{f_2,f_1,f_3\}, \tag{33}$$

etc. It is clear from the relation (5b) that the operator H_U commutes with all P_{jk} ,

$$P_{jk}H_U \subset H_U P_{jk}\,,\quad j,k=1,2,3 \tag{34a}$$

iff the matrix elements of U fulfil $u_{jj}=u_{kk}$ and $u_{jk}=u_{kj}$, i.e., iff U is of the form

$$U = \begin{pmatrix} u & v & v \\ v & u & v \\ v & v & u \end{pmatrix} \tag{34b}$$

for some complex u,v . The unitarity conditions now can be written as

$$|u|^2+2|v|^2 = 1\,, \tag{35a}$$

$$2\,\mathrm{Re}\,\bar{u}v+|v|^2 = 0\,. \tag{35b}$$

The subclass under consideration is parametrized therefore by two real numbers. We want again to characterize the corresponding operators H_U by boundary conditions. They can be chosen as follows

$$\begin{aligned} f_1(0) &= Af'_1(0)+Bf'_2(0)+Bf'_3(0)\,,\\ f_2(0) &= Bf'_1(0)+Af'_2(0)+Bf'_3(0)\,,\\ f_3(0) &= Bf'_1(0)+Bf'_2(0)+Af'_3(0)\,. \end{aligned} \tag{36a}$$

Substituting to these conditions from (5b) and (34b), we get the equations

$$\begin{aligned} 1+u &= -(\bar{\varepsilon}+\varepsilon u)A-2\varepsilon vB\,,\\ v &= -(\bar{\varepsilon}+\varepsilon u)B-\varepsilon vA-\varepsilon vB\,, \end{aligned} \tag{37}$$

which are solved by

$$A = \frac{-\bar{\varepsilon}(1+u+iu+iv+iu^2+iuv-2iv^2)}{(u+2v-i)(1+iu-iv)}\,, \tag{38a}$$

$$B = \frac{i\sqrt{2}\,v}{(u+2v-i)(1+iu-iv)} \tag{38b}$$

provided the common denominator is non-zero. As we have demonstrated, the extensions with continuous wavefunctions are automatically permutation-invariant. It is clear that the conditions (36a) reduce to (6) and (12) if $A=B$, or equivalently $u=v-1$ (cf.(11b)). A tedious but straightforward calculation using repeatedly the conditions (35) shows that $\mathrm{Im}\,A=\mathrm{Im}\,B=0$ so A,B are real numbers. In the same way as above, one can check that the mapping $(u,v)\mapsto(A,B)$ is injective.

It is more difficult to verify directly that every pair of real A,B defines a self-adjoint extension H_U ; it would require to invert the relations (38). Fortunately, there is another way, how to check this statement ; one can use suitable boundary functionals[26] relative to the operator H_0 . Let us define the functionals B_j , $j=1,2,3$, on $D(H_0^*)$ as follows

$$\begin{aligned} B_1(f) &= f_1(0) - Af_1'(0) - Bf_2'(0) - Bf_3'(0) \quad , \\ B_2(f) &= f_2(0) - Bf_1'(0) - Af_2'(0) - Bf_3'(0) \quad , \\ B_3(f) &= f_3(0) - Bf_1'(0) - Bf_2'(0) - Af_3'(0) \quad . \end{aligned} \tag{39}$$

They can be expressed as linear combinations of C_j : $C_j(f)=f_j(0)$ and D_j : $D_j(f)=f_j'(0)$. First we must show that C_j,D_j are boundary functionals relative to the operator H_0 in the sense of Ref.26 . They are defined on $D(H_0^*)$ and $C_j(f)=D_j(f)=0$ for f $D(\overline{H}_0)$; it remains to check their continuity with respect to the graph norm, $\|f\|_*^2 = \|f\|^2+\|H_0 f\|^2$. We shall use the following fact : there is a positive K such that for all $g\in AC^2(\mathbb{R}^+)$, the inequality

$$\int_0^\infty |g'(x)|^2\,dx \;\le\; \int_0^\infty |g''(x)|^2\,dx + K\int_0^\infty |g(x)|^2\,dx \tag{40}$$

holds - cf. Ref.27, Theorem 6.26 . Then for $f=\{f_1,f_2,f_3\}\in D(H_0^*)$, we have

$$|f_j(0)|^2 = -2\,\mathrm{Re}\int_0^\infty f_j(x)\bar f_j'(x)\,dx \le \int_0^\infty |f_j(x)|^2 dx + \int_0^\infty |f_j'(x)|^2 dx \le$$

$$\le (1+K)\int_0^\infty |f_j(x)|^2 dx + \int_0^\infty |f_j''(x)|^2 dx \le (1+K)\|f\|_*^2$$

and similarly

$$|f_j'(0)|^2 \le \int_0^\infty |f_j'(x)|^2 dx + \int_0^\infty |f_j''(x)|^2 dx \le \max(2,K)\|f\|_*^2 \;.$$

By this, the continuity is established. Taking further suitable vectors, e.g., $\varphi_1=\{g,0,0\}$, $\varphi_2=\{0,g,0\}$ and $\varphi_3=\{0,0,g\}$ with $g(x)=\exp(-x^2)$, we see that $\det|B_j(\varphi_k)|\ne 0$ for any A,B , i.e., that the boundary conditions

$$B_j(f) = 0 \quad , \quad j=1,2,3 \tag{36b}$$

are linearly independent. Finally, it is easy to check that the conditions (36) are symmetric for A,B real, i.e., that $B_j(f)=B_j(g)=0$, $j=1,2,3$, implies

$$\{f,g\} \equiv i\sum_{j=1}^{3}\left(f_j(0)\bar g_j'(0) - f_j'(0)\bar g_j(0)\right) = 0 \quad .$$

Then we may apply Theorem XII.4.30 of Ref.26 which asserts that the set of boundary conditions (36) defines a self-adjoint extension of the operator $\overline{H}_0$.

8. The permutation-invariant extensions : exceptional cases

The boundary conditions (36), however, do not exhaust all possible permutation invariant extensions ; the situations when the rhs expressions in (38) are singular must be treated separately. We shall show that there are two one-parameter families and a single extension left.

Consider first the case where $u=i-2v$, i.e., the matrix U is of the form

$$U = \begin{pmatrix} i-2v & v & v \\ v & i-2v & v \\ v & v & i-2v \end{pmatrix} \tag{41a}$$

and the unitarity condition reads

$$2\,\mathrm{Im}\,v - 3|v|^2 = 0 \quad . \tag{41b}$$

The extensions are now characterized by the boundary conditions

$$\begin{aligned} f_1'(0)+f_2'(0)+f_3'(0) &= 0 \quad , \\ f_2(0)-f_3(0) &= C(f_3'(0)-f_2'(0)) \quad , \\ f_1(0)-f_3(0) &= C(f_3'(0)-f_1'(0)) \quad ; \end{aligned} \tag{42a}$$

substituting to them from (5b), we find that

$$C = \frac{3\bar v - \sqrt{2}}{3v} \tag{42b}$$

for a non-zero v . With the help of (41b), it is easy to establish that $\mathrm{Im}\,C=0$ and that (42b) maps the set of complex numbers fulfilling (41b) to the whole real axis.

In a similar way, one can handle the case where the matrix U is of the form

$$U = \begin{pmatrix} v+i & v & v \\ v & v+i & v \\ v & v & v+i \end{pmatrix} \tag{43a}$$

with

$$2\,\mathrm{Im}\,v + 3|v|^2 = 0 \quad . \tag{43b}$$

The boundary conditions are now the following

$$\begin{aligned} f_1'(0) = f_2'(0) = f_3'(0) = f'(0) \quad , \\ f_1(0) + f_2(0) + f_3(0) = Df'(0) \quad , \end{aligned} \tag{44a}$$

where D is a real number related to the matrix (43a) by

$$D = -\frac{3\bar{\varepsilon}v + \sqrt{2}}{v} \tag{44b}$$

provided $v \neq 0$; it can again assume any real value.

There is one more extension left which corresponds to $v = 0$ in (41a) or (43a). The respective boundary conditions can be obtained formally by setting $C = D = \infty$ in (42a) and (44a) ; alternatively, one should use (5b) to check that they are of the form

$$f_1'(0) = f_2'(0) = f_3'(0) = 0 \quad . \tag{45}$$

It is worth mentioning that in view of (11b), none of the exceptional extensions discussed in this section has (all the) wavefunctions continuous at the junction.

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