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P.Exner, P.Šeba

FREE QUANTUM MOTION ON A BRANCHING GRAPH.

The Splitters

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1. Introduction

This is the second part of a paper devoted to study of a free quantum motion on the simplest branching graph, which consists of three half-lines, or "wires", connected in one point. In the first part /1/, hereafter referred to as I , we have constructed all admissible Hamiltonians as the self-adjoint extensions of a suitably chosen non-selfadjoint operator. A particular attention has been paid to the following classes :

(a) the extensions whose domains contain functions continuous at the junction,
(b) the extensions referring to wavefunctions which are continuous only when passing from the first wire to the second one,
(c) the extensions invariant under permutations of the wires ;

each of them has been characterized by appropriate boundary conditions. Now we are going to use these results to construct the S-matrix, or splitter, to each particular extension of the classes (a)-(c) ; we shall point out the cases when the splitters are momentum-independent and/or reflectionless.

Another problem considered here is how the results modify if some of the involved wires is of a finite length. This is important because such three-legged graphs are used as building elements of more complicated structures appearing in the applications. We show that the same boundary conditions can be used as far as we restrict our attention to the extensions which are local in a sense.

Throughout this paper, we use the notation introduced in I as well as the results of the first part freely.

2. Splitters

Now we want to examine what will happen if we take one of the extensions constructed in I as the Hamiltonian of a quantum particle living on the branching graph. It is clear that the particle will move freely except at the junction, and that its behaviour there will depend substantially on the chosen extension. For the sake of brevity, the junction corresponding to a particular extension will be referred to as a splitter.

To each splitter a scattering matrix corresponds, and our aim is now to find these matrices. We shall work in the time independent framework, i.e., we set

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

and demand the vector $f = \{f_1, f_2, f_3\}$ to belong locally to $D(H_U)$, where H_U is the extension under consideration. We are looking for the matrix S, which acts as

$$\underline{a}_{out} = S\underline{a}_{in} \quad , \tag{2}$$

where $\underline{a}_{in}, \underline{a}_{out}$ are column vectors made of $a_{j,in}$ and $a_{j,out}$, respectively. In general, S might depend on the momentum k.

Consider first the case with partially continuous wavefunctions discussed in Sec.I.6. The stated requirement yields the following set of equations

$$\begin{aligned} &a_{1,out} - a_{2,out} = a_{2,in} - a_{1,in} \quad , \\ &(A+ikB)a_{1,out} + ikBa_{2,out} - a_{3,out} = ikBa_{2,in} - (A-ikB)a_{1,in} + a_{3,in} \quad , \\ &(C+ikD)a_{1,out} + ikDa_{2,out} - ika_{3,out} = \\ &\qquad = ikDa_{2,in} - (C-ikD)a_{1,in} - ika_{3,in} \quad . \end{aligned} \tag{3}$$

Solving it, we get the relation (2) with

$$S(k) = [C + ik(2D-A) + 2k^2B]^{-1} \times$$
$$\begin{pmatrix} -C+ikA & 2ik(D-ikB) & -2ik \\ 2ik(D-ikB) & -C+ikA & -2ik \\ 2ik(AD-BC) & 2ik(AD-BC) & -C-ik(2D+A)+2k^2B \end{pmatrix} \tag{4}$$

provided the denominator is non-zero. From what we know about phases of the coefficients (I.29), this might happen only if $A = 2D$ and $C = -2k^2B$, however, such a possibility contradicts to the condition (I.27b). Unitarity of $S(k)$ can be checked by a straightforward way with the help of the conditions (I.27) and (I.30a). Notice that in view of (I.30b), the transposed matrix differs from $S(k)$ by phase factors only.

In what follows, we shall use the term "splitter" for the matrix S as well. Though, in general, it depends on the momentum, some splitters can be k-independent. It is clear that such a situation occurs if $B = C = 0$. The condition (I.27a) then reads $\bar{A}D = -1$ so

$$S = \frac{1}{2+|A|^2}\begin{pmatrix} -|A|^2 & 2 & 2\bar{A} \\ 2 & -|A|^2 & 2\bar{A} \\ 2A & 2A & |A|^2-2 \end{pmatrix} \tag{5a}$$

corresponding to the particular form of the boundary conditions (I.24),

$$\begin{aligned} &f_3(0) = Af_1(0) = Af_2(0) \quad , \\ &f_1'(0) + f_2'(0) = -\bar{A}f_3'(0) \end{aligned} \tag{5b}$$

for any $A \in \mathbb{C}$. Let us remark that the splitters of this type have been used in Ref.I.10. Another interesting subclass consists of reflectionless splitters, i.e., those which have no outgoing wave in the incident "channel". If we choose the wire 1 or 2 as incident, no solution exists within the class specified by the conditions (I.24). There is, of course, the reflectionless splitter with $A = 0$ in (5a), but it is not interesting since it refers to the situation when the third wire is disconnected. On the other hand, the requirement $a_{3,out} = 0$ for $\underline{a}_{in} = (0,0,1)$ leads to $B = C = 0$ and $A = -2D$. Consequently, there is a one-parameter family of reflectionless splitters in this case (when the third wire is taken as incident), namely

$$S(k) = \begin{pmatrix} -\frac{1}{2} & \frac{1}{2} & 2^{-1/2}e^{-i\omega} \\ \frac{1}{2} & -\frac{1}{2} & 2^{-1/2}e^{-i\omega} \\ 2^{-1/2}e^{i\omega} & 2^{-1/2}e^{i\omega} & 0 \end{pmatrix} \tag{6}$$

for a real ω; they refer to the boundary conditions (5b) with $A = \sqrt{2}\,e^{i\omega}$.

The subclass of extensions with fully continuous wavefunctions considered in Sec.I.3 which is described by $A=-D=1$, $B=0$ and $C \in \mathbb{R}$, or by the boundary conditions (I.6) and (I.12), refers to the splitters

$$S(k) = \frac{1}{C-3ik}\begin{pmatrix} -C+ik & -2ik & -2ik \\ -2ik & -C+ik & -2ik \\ -2ik & -2ik & -C+ik \end{pmatrix} . \tag{7}$$

Among them, there is no reflectionless one, and just one which is k-independent, namely that with $C=0$. In the same way, one can treat the n-wire splitter characterized by the boundary conditions (I.14) and (I.19). Solving the corresponding system of linear equations, we get

$$S(k) = \frac{1}{C-nik}\begin{pmatrix} -C+(n-2)ik & -2ik & -2ik & \dots & -2ik \\ -2ik & -C+(n-2)ik & -2ik & \dots & -2ik \\ \dots & \dots & \dots & \dots & \dots \\ -2ik & -2ik & -2ik & \dots & -C+(n-2)ik \end{pmatrix} . \tag{8}$$

Unitarity of this matrix is checked easily. As in the particular case $n=3$, there is no reflectionless splitter, and just one k-independent one which refers to $C=0$.

Let us turn now to the permutation-invariant extensions discussed in Sec.I.7 . The system of equations (3) is now replaced by

$$\begin{aligned}
&(1-ikA)a_{1,out} - ikBa_{2,out} - ikBa_{3,out} = \\
&\qquad = -(1+ikA)a_{1,in} - ikBa_{2,in} - ikBa_{3,in} , \\
&-ikBa_{1,out} + (1-ikA)a_{2,out} - ikBa_{3,out} = \\
&\qquad = -ikBa_{1,in} - (1+ikA)a_{2,in} - ikBa_{3,in} , \\
&-ikBa_{1,out} - ikBa_{2,out} + (1-ikA)a_{3,out} = \\
&\qquad = -ikBa_{1,in} - ikBa_{2,in} - (1+ikA)a_{3,in} .
\end{aligned} \tag{9}$$

Solving it, we find

$$S(k) = \left[1-3ikA+3k^2(B^2-A^2)+ik^3(A^3-3AB^2+2B^3)\right]^{-1} \begin{pmatrix} a & b & b \\ b & a & b \\ b & b & a \end{pmatrix} , \tag{10}$$

where

$$a = -1 + ikA + k^2(B^2-A^2) + ik^3(A^3-3AB^2+2B^3) ,$$

$$b = -2ikB + 2k^2B(B-A) ;$$

it is easy to check that the determinant of the system (9) is non-zero for any real A,B so $S(k)$ makes sense. Unitarity of this matrix verifies directly. Again, there is no reflectionless splitter in the class (10). There is also no k-independent one, except for two limiting cases referring to $A=B$ or $A=-2B$ with $B \to \infty$. However, a brief inspection of the corresponding boundary conditions shows that the first possibility represents the splitter (7) with $C=0$, while the other one refers to the second exceptional class with $D=0$ – cf. (12) below.

Finally, consider the exceptional extensions of Sec.I.8 . By the same procedure as above, we obtain for the first class described by the boundary conditions (I.42a) the following splitter

$$S(k) = \frac{1}{3(1+ikC)}\begin{pmatrix} 3ikC-1 & 2 & 2 \\ 2 & 3ikC-1 & 2 \\ 2 & 2 & 3ikC-1 \end{pmatrix} , \tag{11}$$

which is well defined and unitary for each real C .There is no reflectionless splitter here ; the only k-independent one referring to $C=0$ is identical with (52) for $C=0$ (the two C's are, of course, different). The second class specified by (I.44a) yields similarly

$$S(k) = \frac{1}{3-ikD}\begin{pmatrix} 1-ikD & -2 & -2 \\ -2 & 1-ikD & -2 \\ -2 & -2 & 1-ikD \end{pmatrix} . \tag{12}$$

There is again no reflectionless splitter and one k-independent referring to $D=0$ as mentioned above. The remaining extension (I.45) is easily seen to correspond to $S(k)$ equal to the unit matrix, and therefore k-independent. This case is, however, not interesting because it describes the wires which are disconnected, with Neumann condition at the end of each of them.

3. Wires of a finite length

Description of real experiments requires the knowledge of the electron behaviour on graphs whose lines may be of a finite length. In fact the semiinfinite wires suit usually only as an idealized description of the external leads. The simplest non-trivial graph of this type is sketched on Fig.1, where each l_j is either a positive number or infinity ; it can be used, of course, as a building element of more complicated graphs.

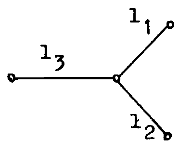

Fig.1 Connection of three wires - general case.

In order to describe a free quantum motion on such a graph, one has to proceed as in I . In the relation (I.1), $L^2(\mathbb{R}^+)$ is replaced now by $L^2(0,l_j)$. The construction starts with the operator H_0 defined by the relations (I.2), where, however, $D(H_{0,j}) = C_0^{\infty}(0,l_j)$ or any other dense subset of $AC^2(0,l_j)$ containing the functions with $f_j(0) = f_j'(0) = f_j(l_j) = f_j'(l_j) = 0$. The deficiency indices of this operator are $(3+f, 3+f)$, where f is the number of finite-length wires, and therefore we have many more self-adjoint extensions than in the case $f = 0$. Fortunately, not each of them is interesting. We restrict our attention to the Hamiltonians H_U obtained by extensions of H_0 which are <u>local</u> in the sense that

$$\operatorname{supp} H_U f \subset \operatorname{supp} f \tag{13}$$

for all $f \in D(H_U)$; the support of a vector $f \in \mathcal{H}$ is naturally defined as Cartesian product of the supports of the functions f_j .

Such extensions can be constructed with the help of separated boundary conditions. We fix the behaviour of wavefunctions on the loose ends of the finite-length wires by standard boundary conditions

$$f_j(l_j)\cos\alpha_j + f_j'(l_j)\sin\alpha_j = 0 \tag{14}$$

for some real α_j . On the other hand, for behaviour at the junction we can choose one of the following possibilities :

(a) the boundary conditions (I.6) and (I.12),
(b) the conditions (I.24),
(c) the conditions (I.36), or (I.42a), or (I.44a), or (I.45) .

In the same way as in Sec.I.7, one can check that together we have a set of $3+f$ boundary conditions, which are linearly independent

and symmetric, and define therefore a self-adjoint extension of H_0 .

In the cases (a) and (b), those extensions are distinguished in the same way as in I , namely by the full or partial continuity of the wavefunctions. The third case requires a brief explanation. One cannot speak now about the permutation symmetry unless the wires are of the same length and $\alpha_1 = \alpha_2 = \alpha_3$ in (14). Nevertheless, any extension H_U of the class (c) remains <u>locally permutation-invariant</u> in the following sense : if $f \in D(H_U)$ has $\operatorname{supp} f \subset [0,l] \times [0,l] \times [0,l]$, where $l \leq \min_{1\leq j\leq 3} l_j$, then $P_{jk} f \in D(H_U)$ and $P_{jk} H_U f = H_U P_{jk} f$ for each $j,k = 1,2,3$. One might say, that the particle whose evolution is governed by some of the extensions of the class (c) does not distinguish the wires when it is close to the junction.

The described method based on adaptation of the "semiinfinite" results has a drawback. One cannot prove that we have obtained all extensions of a given class, e.g., all locally permutation-invariant extensions in the case (c), without returning to the deficiency functions. The latter are now more complicated, however, being combinations of two exponential functions with the coefficients depending on α_j and l_j .

Since the above described extensions are specified by the same boundary conditions as in the semiinfinite case, one can use the splitters found in the preceding section when treating the scattering problem on a branching graph. Of course, not every graph is suitable for this purpose. In the system of three wires, the scattering problem can be formulated if two of them are semiinfinite. If the third wire is of a finite length, we obtain an interesting situation ; one can study how the energy eigenvalues for the particle living on the interval disjoint from the line turn to resonances when we "tune" the junction by changing the parameters specifying the used self-adjoint extension. Up to our knowledge, such experiments have not been performed but they are fully conceivable with the technology used for fabrication of the metallic rings.

However, the splitters derived in the preceding section can be used for analysis of the scattering problem on a more complicated graph, if only the latter is composed of two or more three-legged parts. The simplest example is represented by a ring with two semiinfinite leads ; in this case we need two splitters to describe behaviour of the wavefunctions at the junctions. This problem will be discussed in a subsequent paper.

References

The full list of them has been given in I; here we refer to:

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Экснер П., Шеба П. E2-87-214
Свободное квантовое движение на разветвляющемся графике. Расщепители

Мы рассматриваем свободное квантовое движение на графике, состоящем из трех полупрямых, концы которых соединены. Для каждого из допустимых гамильтонианов, построенных в первой части этой работы, мы вычисляем здесь S-матрицу, которая описывает рассеяние на контакте; мы выделяем те случаи, в которых S-матрица не зависит от импульса и/или описывает рассеяние без отражения. Обсуждается также случай, когда некоторые ветви графика имеют конечную длину. Результаты могут быть использованы например для описания недавних измерений проводимости крошечных металлических колец.

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Free Quantum Motion on a Branching Graph. The Splitters

We consider free quantum motion of a quantum particle on the graph consisting of three halflines whose ends are connected. For each of the admissible Hamiltonians constructed in the first part of this paper, we calculate here the S-matrix which describes scattering on the junction; we point out the cases in which the S-matrix is momentum-independent and/or reflectionless. We discuss also the case when some branches of the graph are of a finite length. The results can be used, e.g., for description of recent conductivity measurements on tiny metallic rings.

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

Communication of the Joint Institute for Nuclear Research. Dubna 1987