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Symmetries and parametrization of the transfer matrix in electronic quantum transport theory (*)

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Résumé. — Nous analysons pour les cas orthogonal, unitaire et symplectique, la structure de l'espace où est définie la matrice de transfert multiplicative d'un diffuseur élastique à N canaux. Nous décrivons cet espace à l'aide de N paramètres radiaux, dont la conductance est une fonction simple, et par deux matrices unitaires auxiliaires dont la structure dépend de la classe d'universalité.

Abstract. — We analyze for the orthogonal, unitary and symplectic cases the structure of the space where the multiplicative transfer matrix M of a multi-channel elastic scatterer is defined. We parametrize this space with a set of radial parameters, which are related in a simple way to the conductance of the elastic scatterer, and with two auxiliary unitary matrices, whose structure depends on the universality class.

1. Introduction.

The importance of basic symmetry considerations (time reversal symmetry and spin rotation symmetry) has been appreciated for a long time in electronic quantum transport theory [1]. In the absence of sufficient spin-orbit scattering, the spin-up and spin-down electronic gases are decoupled in a non-interacting theory. One can then ignore the electronic spins, except for a trivial twofold degeneracy which can be removed by an applied magnetic field B (Zeemann splitting). A spinless-particle theory is then sufficient in order to describe quantum transport, and two cases can occur: either the system is time reversal invariant (*orthogonal case*) or this symmetry is removed by an applied magnetic field (*unitary case*). In the presence of strong spin-orbit scattering, spin components are coupled and a spin-1/2-particle theory is then necessary; two cases can also occur: in the presence of time reversal symmetry one has the *symplectic case* and the removal of this last symmetry by a magnetic field gives again the unitary case.

The above classification in three cases was first introduced by Dyson [2] very generally for

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quantum mechanical ensembles and yields [1] three different renormalization group β -functions for electronic quantum transport. The importance of transitions between these three cases is well understood for the weak-localization corrections in the metallic regime ($k_F \ell > 1$), as well as for the magnitude of the universal conductance fluctuations, but has been realized only very recently for the localized regime ($k_F \ell < 1$), where the magnitude of the localization length is changed when a symmetry is broken [3].

Therefore, a theory where symmetry considerations are carefully taken into account from the beginning is of primary interest. Two random matrix approaches introducing maximum entropy ensembles for the multiplicative transfer matrix M have been based on this point of view (see Refs. [4-6] for reviews). The first one [7-12] uses the parametrization of M that we will demonstrate in this paper; i.e.

$$M = U \begin{pmatrix} \sqrt{1+\lambda} & \sqrt{\lambda} \\ \sqrt{\lambda} & \sqrt{1+\lambda} \end{pmatrix} V, \quad (1.1)$$

where λ is a diagonal, real, positive matrix and U and V are unitary matrices whose structure depends on the universality class. The second one [13, 15] is based more specifically on the matrix

$$X = \frac{1}{4} [M^\dagger M + (M^\dagger M)^{-1} - 2], \quad (1.2)$$

which turns out to be diagonalizable as

$$X = V^\dagger \begin{pmatrix} \lambda & 0 \\ 0 & \lambda \end{pmatrix} V. \quad (1.3)$$

We note that the study of the parametrization (1.1), which is a natural generalization of Bargmann's parametrization [16] of M for a many-channel system, gives us also the structure of the eigenvectors of X . We recall that the interest of formulas (1.1) and (1.3) consists in introducing the matrix λ , whose diagonal elements $\{\lambda_a\}$ are simply related to the two-probe conductance [4] by

$$g = 2 \sum_{a=1}^N \frac{1}{1 + \lambda_a} \quad (1.4)$$

In order to understand the effect of symmetry breaking, we have to know the structure of the matrices U and V for the three universality cases. This will allow us to know in which *a priori* matrix space M and X are defined for a given symmetry and how this space is either enlarged or restricted when a basic symmetry is removed. A full description of the transition between different universality classes would suppose a knowledge of how the probability density of M (or X) diffuses from one space of definition to another, when a symmetry breaking perturbation is applied. One could think, for instance, of applying a Brownian motion model in order to describe this diffusion [17], but we think useful, as a first step, to give in this work a careful and rigorous study of the three different spaces of definition of M (or X), with the corresponding appropriate parametrization.

The parametrization demonstrated in the present paper was used without proof in some of the earlier publications indicated above. Thus we first review the results that were used in those references, both for the sake of completeness and to indicate more specifically the statements that we want to prove or extend in the following sections.

Suppose that the disordered system is placed between two perfect leads: in the latter, the quantized transverse states define N channels for propagating modes, so that the one-particle

wave function is specified by $2N$ or $4N$ components, depending on whether the particle has no spin or spin $1/2$, respectively. The transfer matrix M relates the vector on the right of the system with that on the left. The requirement of flux conservation and, in the absence of a magnetic field, that of time-reversal symmetry, impose restrictions among the matrix elements of M . The question then arises as to how one can write M in terms of independent parameters.

Consider spinless particles. We write the wave function on the left and on the right of the disordered system, respectively, as

$$\Psi(x) = (\Psi_1(x), \dots, \Psi_N(x)) \quad (1.5a)$$

$$\Psi'(x) = (\Psi'_1(x), \dots, \Psi'_N(x)). \quad (1.5b)$$

To be specific, suppose that the basic solutions in the perfect conductors are plane waves. The n -th component can then be expressed as a linear combination of unit-flux plane waves travelling to the right and to the left; i.e.

$$\Psi_n(x) = a_n \frac{e^{ik_n x}}{(\hbar k_n/m)^{1/2}} + b_n \frac{e^{-ik_n x}}{(\hbar k_n/m)^{1/2}}. \quad (1.6a)$$

$$\Psi'_n(x) = a'_n \frac{e^{ik_n x}}{(\hbar k_n/m)^{1/2}} + b'_n \frac{e^{-ik_n x}}{(\hbar k_n/m)^{1/2}}. \quad (1.6b)$$

The transfer matrix M relates the $2N$ coefficients appearing in $\Psi_n(x)$ of (1.6a) with those appearing in $\Psi'_n(x)$ of (1.6b); i.e.

$$C' = MC, \quad (1.7)$$

where

$$C = \begin{pmatrix} a \\ b \end{pmatrix}, \quad C' = \begin{pmatrix} a' \\ b' \end{pmatrix} \quad (1.8a, b)$$

$$M = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \quad (1.8c)$$

where a, b, a', b' are N -dimensional vectors and $\alpha, \beta, \gamma, \delta, N \times N$ matrices.

The requirement of flux conservation imposes on M the restriction

$$M \Sigma_z M^\dagger = \Sigma_z \quad (1.9a)$$

or, equivalently,

$$M^\dagger \Sigma_z M = \Sigma_z \quad (1.9b)$$

where

$$\Sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (1.10)$$

is the $2N$ -dimensional generalization of the usual Pauli matrix σ_x , 1 being the $N \times N$ unit matrix. We thus see that the transfer matrices M satisfying flux conservation form the pseudounitary group $U(N, N)$; the number ν of independent parameters is given by

$$\nu = (2N)^2, \quad (1.11)$$

just as for the unitary group $U(2N)$. As in references [14, 15], one can perform the unitary transformation

$$P = U_0^\dagger M U_0, \quad (1.12)$$

where

$$U_0 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \\ -i & 1 \end{pmatrix}, \quad (1.13)$$

and show that the new matrices P satisfy the relation

$$P^\dagger J P = J \quad (1.14)$$

where

$$J = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}. \quad (1.15)$$

If, in addition, the Hamiltonian governing the system is invariant under the operation of time reversal (the *orthogonal case*), our transfer matrices M must also satisfy the requirement

$$M^* = \Sigma_x M \Sigma_x. \quad (1.16)$$

It can be checked that the condition (1.16) implies that the P matrices of (1.12) must be real,

$$P = P^*, \quad (1.17)$$

so that (1.14) define the real symplectic group $\text{Sp}(2N, R)$, with

$$\nu' = N(2N + 1) \quad (1.18)$$

independent parameters.

In reference [12] it was indicated without proof that any M -matrix satisfying the flux-conservation requirement (1.9) can be parameterized as (see (1.1))

$$M = \begin{bmatrix} u^{(1)} & 0 \\ 0 & u^{(3)} \end{bmatrix} \begin{bmatrix} \sqrt{1+\lambda} & \sqrt{\lambda} \\ \sqrt{\lambda} & \sqrt{1+\lambda} \end{bmatrix} \begin{bmatrix} u^{(2)} & 0 \\ 0 & u^{(4)} \end{bmatrix} = U \Gamma V, \quad (1.19)$$

where $u^{(i)}$ ($i = 1, \dots, 4$) are arbitrary $N \times N$ unitary matrices and λ is a real, diagonal matrix with non-negative elements $\lambda_1, \dots, \lambda_N$.

The T-symmetry requirement (1.16) imposes the additional constraints

$$u^{(3)} = (u^{(1)})^*, \quad u^{(4)} = (u^{(2)})^* \quad (1.20)$$

In this latter case, $u^{(1)}$ and $u^{(2)}$ give rise to N^2 parameters each, and λ to N additional ones, in agreement with (1.18). For $N = 1$, we get back Bargmann's result [16].

In the absence of T-symmetry, (1.19) contains $4N^2 + N$ parameters, N more than in (1.11). This is connected with the fact that, when all λ_a 's are non degenerate, the M of (1.19) is insensitive to the transformation

$$U \rightarrow UG, \quad V \rightarrow G^{-1}V, \quad (1.21a)$$

G being the diagonal matrix

$$G = \begin{bmatrix} d & 0 \\ 0 & d \end{bmatrix}, \quad (1.21b)$$

with

$$d = \begin{bmatrix} e^{i\eta_1} & & & \\ & & 0 & \\ & & & \\ & 0 & & \\ & & & e^{i\eta_N} \end{bmatrix}, \tag{1.21c}$$

so that (1.21) could be used to eliminate N parameters in the $u^{(i)}$ of (1.19).

The above are, basically, the results used in references [8-12]. Equations (1.19)-(1.21) are the ones we shall be particularly interested in in what follows. The purpose of the next section of the present paper is to give a proof of the parametrization (1.19), (1.20) : we start with the *orthogonal* case, because the extra freedom (1.21) occurring in the unitary case is absent and, in that sense, the analysis is a bit simpler. In section 3 we then study the unitary case : i.e., we prove the parametrization of equation (1.19) and analyze the freedom (1.21) more closely. Finally, extension to spin-1/2 particles — the *symplectic* case — is dealt with in section 4.

2. The orthogonal case (Particles with no spin, satisfying the conditions of flux conservation and T-symmetry).

The T-symmetry condition (1.16) implies that the transfer matrix M of (1.8c) can be written as

$$M = \begin{pmatrix} \alpha & \beta \\ \beta^* & \alpha^* \end{pmatrix}, \tag{2.1}$$

while the requirement of flux conservation (1.9a) or (1.9b) imposes on α, β the restrictions [8]

$$\alpha \alpha^\dagger - \beta \beta^\dagger = 1 \tag{2.2}$$

$$\alpha \beta^T = \beta \alpha^T, \tag{2.3}$$

or

$$\alpha^\dagger \alpha - \beta^T \beta^* = 1 \tag{2.4}$$

$$\alpha^\dagger \beta = \beta^T \alpha^*, \tag{2.5}$$

respectively.

The purpose of this section is to express in terms of independent parameters the most general matrices α, β that occur in (2.1) and satisfy the conditions (2.2)-(2.5). We write α, β in their « polar representation » [18]

$$\alpha = u \ell v \tag{2.6}$$

$$\beta = u' \ell' v' \tag{2.7}$$

All the matrices occurring in (2.6), (2.7) are $N \times N$: u, v, u', v' are unitary and ℓ, ℓ' are diagonal, real and positive (any phase appearing in ℓ, ℓ' can be incorporated in u, v).

The diagonal matrix appearing in the polar representation is unique : for instance, ℓ in (2.6) contains the positive square root of the eigenvalues of the Hermitean matrix

$$h = \alpha \alpha^\dagger. \tag{2.8}$$

In contrast, the unitary matrices u, v are not unique : suppose that ℓ has the structure ⁽¹⁾

$$\ell = \begin{bmatrix} \ell_1 I_{n_1} & & & \\ & & 0 & \\ & & & \\ & 0 & & \\ & & & \ell_k I_{n_k} \end{bmatrix} \quad (2.9)$$

where I_{n_i} is the $n_i \times n_i$ unit matrix, ℓ_i are positive numbers and $\sum_{i=1}^k n_i = N$; then the transformation

$$u \rightarrow ud, \quad v \rightarrow d^{-1}v, \quad (2.10)$$

d having the structure

$$d = \begin{bmatrix} u_1 & & & \\ & & 0 & \\ & & & \\ & 0 & & \\ & & & u_k \end{bmatrix} \quad (2.11)$$

(u_i ($i = 1, \dots, k$) are unitary $n_i \times n_i$ matrices), leaves α of (2.6) invariant : this is so because d of (2.11) and ℓ of (2.9) commute and hence

$$\alpha = ulv \rightarrow udl d^{-1}v = ulv. \quad (2.12)$$

If there is no degeneracy in (2.9) (i.e. $n_a = 1, a = 1, \dots, N$), then, in (2.11), $u_a = \exp(i\phi_a)$ and the nonuniqueness mentioned above is related to these N phases.

In any case, given one form of writing α (i.e. with one u, v in (2.6)), we ask what are the most general u', v', ℓ' of (2.7) that satisfy equations (2.2)-(2.5).

Substitution of (2.6) and (2.7) in (2.2)-(2.5) yields

$$u\ell^2 u^\dagger - u' \ell'^2 u'^\dagger = 1 \quad (2.13)$$

$$ulvv'^\dagger \ell' u'^\dagger = u' \ell' v'v'^\dagger \ell u^\dagger \quad (2.14)$$

$$v^\dagger \ell^2 v - v'^\dagger \ell'^2 v'^* = 1 \quad (2.15)$$

$$v^\dagger \ell u^\dagger u' \ell' v' = v'^\dagger \ell' u'^\dagger u^* \ell v^* \quad (2.16)$$

One solution to these equations is clearly

$$u' = u, \quad v' = v^*, \quad \ell'^2 = \ell^2 - 1, \quad (2.17)$$

which implies

$$\alpha = ulv \quad (2.18)$$

$$\beta = u \sqrt{\ell^2 - 1} v^* \quad (2.19)$$

(1) The n_i degenerate eigenvalues ℓ_i may not appear next to each other as in (2.9), but scattered along the diagonal ; however, one can always bring them together by means of a suitable permutation matrix that can be incorporated in u, v . We shall thus keep the structure of ℓ as in (2.9).

Defining

$$\ell = \sqrt{1 + \lambda} \tag{2.20}$$

we then have

$$M = \begin{pmatrix} u & 0 \\ 0 & u^* \end{pmatrix} \begin{pmatrix} \sqrt{1 + \lambda} & \sqrt{\lambda} \\ \sqrt{\lambda} & \sqrt{1 + \lambda} \end{pmatrix} \begin{pmatrix} v & 0 \\ 0 & v^* \end{pmatrix}, \tag{2.21}$$

which has the form of equation (1.19) with (1.20).

We should keep in mind that (2.17) is just one solution of (2.13)-(2.16) and by no means we know whether any transfer matrix M can be written as in (2.21) (in the orthogonal case). We now proceed to find the *most general* solution.

From equation (2.13) we have

$$(u'^{\dagger} u) (\ell^2 - 1) (u'^{\dagger} u)^{\dagger} = \ell'^2 \tag{2.22}$$

We apply the lemma of the Appendix, with $\mu = \ell^2 - 1$ having the structure (2.9). Equations (A7) and (A6) then give

$$\ell = P \sqrt{\ell^2 - 1} P^{\text{T}} \tag{2.23}$$

$$u' = u d_1^{\dagger} P^{\text{T}}, \tag{2.24}$$

where d_1 has the structure (2.11).

From equation (2.15) we have

$$(v'^* v^{\dagger}) (\ell^2 - 1) (v'^* v^{\dagger})^{\dagger} = \ell'^2 \tag{2.25}$$

We apply the lemma of the appendix ; again, P takes $\sqrt{\ell^2 - 1}$ into ℓ' , as in (2.23). Equation (A6) then gives

$$v' = P d_2^* v^*, \tag{2.26}$$

where d_2 has the structure (2.11).

We now substitute (2.23)-(2.26) in (2.14), with the result (which coincides with that obtained upon substituting in (2.16))

$$d_2^{\dagger} d_1^* = d_1^{\dagger} d_2^* \equiv s = s^{\text{T}}, \tag{2.27}$$

s being a unitary, symmetric matrix with the structure (2.11).

Therefore, given α in the form (2.6), substitution of (2.23)-(2.27) in (2.7) and use of the fact that d_1, d_2 commute with ℓ (see Eqs. (2.9) and (2.11)) shows that the most general β satisfying (2.2)-(2.5) is

$$\beta = u s \sqrt{\ell^2 - 1} v^* \tag{2.28}$$

Any unitary and symmetric matrix s can be written as

$$s = w w^{\text{T}}, \tag{2.29}$$

where w is unitary ; s and w have the structure (2.11), so that they commute with ℓ , which has the structure (2.9). Then

$$\beta = (u w) \sqrt{\ell^2 - 1} (w^{\dagger} v)^* \tag{2.30}$$

Now we can make use of the arbitrariness in the u, v of (2.6) explained right after (2.8) to write α as

$$\alpha = u \ell v = (uw) \ell (w^\dagger v). \quad (2.31)$$

Defining

$$u^{(1)} = uw, \quad u^{(2)} = w^\dagger v, \quad \ell^2 = 1 + \lambda, \quad (2.32)$$

we can write

$$M = \begin{pmatrix} u^{(1)} & 0 \\ 0 & u^{(1)*} \end{pmatrix} \begin{pmatrix} \sqrt{1+\lambda} & \sqrt{\lambda} \\ \sqrt{\lambda} & \sqrt{1+\lambda} \end{pmatrix} \begin{pmatrix} u^{(2)} & 0 \\ 0 & u^{(2)*} \end{pmatrix}, \quad (2.33)$$

which has precisely the structure found in (2.21), or (1.19) with (1.20).

In conclusion, we have proved that, *in the orthogonal case, any transfer matrix M can be written in the form (2.33).*

We now inquire whether the decomposition (2.33) is unique. To answer this question we need to know whether there is a transformation of the type

$$u^{(1)} \rightarrow u^{(1)} u_0, \quad u^{(2)} \rightarrow u'_0 u^{(2)} \quad (2.34)$$

that leaves M invariant. Clearly, this can only happen if u_0 and u'_0 are of the form (2.11); i.e.

$$u^{(1)} \rightarrow u^{(1)} d_1, \quad u^{(2)} \rightarrow d_2 u^{(2)} \quad (2.35)$$

because then d_1, d_2 commute with λ of (2.33), which has the structure (2.9).

For M to remain invariant we need

$$d_1 d_2 = 1 \quad (2.36)$$

$$d_1 d_2^* = 1, \quad (2.37)$$

which imply

$$d_1 = d_1^* \quad (2.38)$$

$$d_2 = d_2^* = d_1^T. \quad (2.39)$$

Therefore, if d has the form (2.11) and is *real* and *orthogonal*, the transformation

$$u^{(1)} \rightarrow u^{(1)} d, \quad u^{(2)} \rightarrow d^T u^{(2)} \quad (2.40)$$

leaves M invariant. Therefore, *the decomposition (2.33) has the arbitrariness expressed by (2.40). In particular, if the λ_i 's are nondegenerate, the decomposition is unique.*

3. The unitary case (Particles with no spin, satisfying the condition of flux conservation).

We now drop the condition of T-symmetry used in the previous section.

The flux-conservation requirement (1.9a) or (1.9b) imposes on $\alpha, \beta, \gamma, \delta$ of (1.8c) the restrictions

$$\alpha \alpha^\dagger - \beta \beta^\dagger = 1 \quad (3.1)$$

$$\delta \delta^\dagger - \gamma \gamma^\dagger = 1 \quad (3.2)$$

$$\alpha \gamma^\dagger = \beta \delta^\dagger \quad (3.3)$$

or

$$\alpha^\dagger \alpha - \gamma^\dagger \gamma = 1 \tag{3.4}$$

$$\delta^\dagger \delta - \beta^\dagger \beta = 1 \tag{3.5}$$

$$\alpha^\dagger \beta = \gamma^\dagger \delta . \tag{3.6}$$

We write $\alpha, \beta, \gamma, \delta$ in their polar representation

$$\alpha = u\ell v, \quad \beta = u' \ell' v' \tag{3.7a, b}$$

$$\gamma = x' m' y', \quad \delta = xmy . \tag{3.8a, b}$$

All the matrices occurring in (3.7), (3.8) are $N \times N$: $u, v, u', v', x, y, x', y'$ are unitary and ℓ, ℓ', m, m' are diagonal, real and positive.

Substituting (3.7), (3.8) in (3.1)-(3.6) we get

$$u\ell^2 u^\dagger - u' \ell'^2 u'^\dagger = 1 \tag{3.9}$$

$$xm^2 x^\dagger - x' m'^2 x'^\dagger = 1 \tag{3.10}$$

$$u\ell v y'^\dagger m' x'^\dagger = u' \ell' v' y^\dagger m x^\dagger \tag{3.11}$$

$$v^\dagger \ell^2 v - y'^\dagger m'^2 y' = 1 \tag{3.12}$$

$$y^\dagger m^2 y - v'^\dagger \ell'^2 v' = 1 \tag{3.13}$$

$$v^\dagger \ell u^\dagger u' \ell' v' = y'^\dagger m' x'^\dagger xmy . \tag{3.14}$$

Suppose we are given u, ℓ, v, x, y . One solution (for $u', \ell', v', x', m', y', m$) of equations (3.9)-(3.14) is clearly

$$u' = u, \quad x' = x, \quad v' = y, \quad y' = v \tag{3.15a, b, c, d}$$

$$\ell' = \sqrt{\ell^2 - 1}, \quad m' = \sqrt{\ell^2 - 1}, \quad m = \ell, \tag{3.15e, f, g}$$

which implies

$$\alpha = u\ell v, \quad \beta = u \sqrt{\ell^2 - 1} y \tag{3.16}$$

$$\gamma = x \sqrt{\ell^2 - 1} v, \quad \delta = x\ell y$$

and, with $\ell = \sqrt{1 + \lambda}$,

$$M = \begin{bmatrix} u & 0 \\ 0 & x \end{bmatrix} \begin{bmatrix} \sqrt{1 + \lambda} & \sqrt{\lambda} \\ \sqrt{\lambda} & \sqrt{1 + \lambda} \end{bmatrix} \begin{bmatrix} v & 0 \\ 0 & y \end{bmatrix}, \tag{3.17}$$

which has the structure of equation (1.19).

At this stage of the analysis we do not know whether *any* transfer matrix can be written, in the unitary case, as in (3.17). Thus we now look for the general solution.

From (3.9) we have

$$(u'^\dagger u) (\ell^2 - 1) (u'^\dagger u)^\dagger = \ell'^2 \tag{3.18}$$

We apply the lemma of the Appendix, with $\mu = \ell^2 - 1$ having the structure (2.9). Equations (A7) and (A6) then give

$$\ell' = P_1 \sqrt{\ell^2 - 1} P_1^\dagger \tag{3.19}$$

$$u' = u d_1^\dagger P_1^\dagger, \tag{3.20}$$

where d_1 has the structure (2.11).

From (3.12) we have

$$(y' v^\dagger) (\ell^2 - 1) (v y'^\dagger) = m'^2 \quad (3.21)$$

We apply again the lemma of the Appendix, to get

$$m' = P_2 \sqrt{\ell^2 - 1} P_2^\dagger \quad (3.22)$$

$$y' = P_2 d_2 v \quad (3.23)$$

where d_2 has the structure (2.11).

From (3.10) and using (3.22) we have

$$(x^\dagger x' P_2) \ell^2 (x^\dagger x' P_2)^\dagger = m^2 \quad (3.24)$$

Again ℓ^2 has the structure (2.9). The lemma gives

$$m = P_3 \ell P_3^\dagger \quad (3.25)$$

and

$$x' = x P_3 d_3 P_2^\dagger, \quad (3.26)$$

where d_3 has the structure (2.11).

From (3.13) and using (3.19) and (3.25) we have

$$(P_1^\dagger v' y^\dagger P_3) \ell^2 (P_3^\dagger y v'^\dagger P_1) = \ell^2, \quad (3.27)$$

so that

$$v' = P_1 d_4 P_3^\dagger y, \quad (3.28)$$

where d_4 has the structure (2.11).

We now substitute (3.19)-(3.28) in (3.11), with the result (which coincides with that obtained upon substituting in (3.14))

$$d_2^\dagger d_3^\dagger = d_1^\dagger d_4 \equiv d_0. \quad (3.29)$$

Summarizing, given u, ℓ, v, x, y , the most general solution of (3.9)-(3.14) for the remaining matrices (to be contrasted with the particular solution (3.15)) is given by

$$u' = u d_1^\dagger P_1^\dagger, \quad x' = x P_3 d_3 P_2^\dagger, \quad v' = P_1 d_4 P_3^\dagger y, \quad y' = P_2 d_2 v \quad (3.30a, b, c, d)$$

$$\ell' = P_1 \sqrt{\ell^2 - 1} P_1^\dagger, \quad m' = P_2 \sqrt{\ell^2 - 1} P_2^\dagger, \quad m = P_3 \ell P_3^\dagger, \quad (3.30e, f, g)$$

with ℓ having the structure (2.9) and d_1, d_2, d_3, d_4 the structure (2.11) satisfying (3.29).

With $\ell = \sqrt{1 + \lambda}$, we can then write $\alpha, \beta, \gamma, \delta$ as

$$\alpha = u \sqrt{1 + \lambda} v, \quad \beta = u \sqrt{\lambda} d_0 P_3^\dagger y \quad (3.31a, b)$$

$$\gamma = x P_3 d_0^\dagger \sqrt{\lambda} v, \quad \delta = x P_3 d_0^\dagger \sqrt{1 + \lambda} d_0 P_3^\dagger y. \quad (3.31c, d)$$

If we define

$$u^{(1)} = u, \quad u^{(2)} = v, \quad u^{(3)} = xP_3 d_0^\dagger, \quad u^{(4)} = d_0 P_3^\top y, \quad (3.32)$$

We can finally write M as

$$M = \begin{pmatrix} u^{(1)} & 0 \\ 0 & u^{(3)} \end{pmatrix} \begin{pmatrix} \sqrt{1+\lambda} & \sqrt{\lambda} \\ \sqrt{\lambda} & \sqrt{1+\lambda} \end{pmatrix} \begin{pmatrix} u^{(2)} & 0 \\ 0 & u^{(4)} \end{pmatrix} \equiv U F V, \quad (3.33)$$

which has precisely the structure found in (3.17), or (1.19).

In conclusion, we have proved that, *in the unitary case, any transfer matrix M can be written in the form (3.33).*

There only remains to study the uniqueness of the decomposition (3.33). Just as in the previous section, we need to know whether there is a transformation

$$\begin{aligned} u^{(1)} &\rightarrow u^{(1)} u_0^{(1)}, & u^{(2)} &\rightarrow u_0^{(2)} u^{(2)} \\ u^{(3)} &\rightarrow u^{(3)} u_0^{(3)}, & u^{(4)} &\rightarrow u_0^{(4)} u^{(4)} \end{aligned} \quad (3.34)$$

that leaves $\alpha, \beta, \gamma, \delta$ invariant. Clearly this can only happen if $u_0^{(1)}, u_0^{(2)}, u_0^{(3)}, u_0^{(4)}$ are of the form (2.11); i.e.

$$\begin{aligned} u^{(1)} &\rightarrow u^{(1)} d^{(1)}, & u^{(2)} &\rightarrow d^{(2)} u^{(2)} \\ u^{(3)} &\rightarrow u^{(3)} d^{(3)}, & u^{(4)} &\rightarrow d^{(4)} u^{(4)}, \end{aligned} \quad (3.35)$$

because then the $d^{(i)}$ commute with λ which has the structure (2.9).

Invariance of $\alpha, \beta, \gamma, \delta$ implies, respectively

$$d^{(1)} d^{(2)} = 1 \quad (3.36a)$$

$$d^{(1)} d^{(4)} = 1 \quad (3.36b)$$

$$d^{(3)} d^{(2)} = 1 \quad (3.36c)$$

$$d^{(3)} d^{(4)} = 1. \quad (3.36d)$$

Equations (3.36a, b) give

$$d^{(2)} = d^{(4)} = (d^{(1)})^\dagger \quad (3.37a)$$

Equations (3.36c, d) give

$$d^{(2)} = d^{(4)} = (d^{(3)})^\dagger \quad (3.37b)$$

Therefore

$$d^{(1)} = d^{(3)}, \quad d^{(2)} = d^{(4)} = (d^{(1)})^\dagger \quad (3.38)$$

I.e., if

$$G = \begin{pmatrix} d & 0 \\ 0 & d \end{pmatrix} \quad (3.39)$$

(see Eq. (1.18)), with d having the structure (2.11), then $M = U F V$ remains invariant if

$$U \rightarrow U G, \quad V \rightarrow G^\dagger V. \quad (3.40)$$

Therefore, *the decomposition (3.33) has the arbitrariness expressed by (3.40)*. In particular, *if the λ_i 's are nondegenerate,*

$$d = \begin{bmatrix} e^{i\eta_1} & & & \\ & & 0 & \\ & 0 & & \\ & & & e^{i\eta_N} \end{bmatrix}, \quad (3.41)$$

and even in that case *the decomposition (3.33) is not unique*. This has to be contrasted with the uniqueness of the decomposition in the orthogonal case, when the λ_i 's are nondegenerate.

4. The symplectic case (Particles with spin 1/2, satisfying the condition of flux conservation and T-symmetry).

The coefficients appearing in equation (1.6) now have an extra index \pm that specifies the spin projection ; i.e.

$$\begin{aligned} a_{1+} &\rightarrow \rightarrow a'_{1+} \\ a_{1-} &\rightarrow \rightarrow a'_{1-} \\ &\cdot \\ a_{N+} &\rightarrow \rightarrow a'_{N+} \\ a_{N-} &\rightarrow \rightarrow a'_{N-} \end{aligned} \quad (4.1)$$

$$\begin{aligned} b_{1+} &\leftarrow \leftarrow b'_{1+} \\ b_{1-} &\leftarrow \leftarrow b'_{1-} \\ &\cdot \\ b_{N+} &\leftarrow \leftarrow b'_{N+} \\ b_{N-} &\leftarrow \leftarrow b'_{N-} \end{aligned}$$

The $4N \times 4N$ transfer matrix M is defined as in (1.7), (1.8), where a and b now denote $2N$ -dimensional vectors.

Time-reversal invariance implies that if $\begin{pmatrix} a \\ b \end{pmatrix}$ is a solution, $\vartheta \begin{pmatrix} a \\ b \end{pmatrix}$ is a solution too, ϑ being the time-reversal operator

$$\vartheta = i\sigma_y C. \quad (4.2)$$

Here, C is the complex conjugation operator and the Pauli matrix σ_y acts on the indices \pm introduced above. The consequence of T-symmetry, i.e. the equivalent of equation (1.16) is now

$$M^* = KMK^T, \quad (4.3)$$

where

$$K = \begin{pmatrix} 0 & k \\ k & 0 \end{pmatrix}. \quad (4.4)$$

Here, k is the $2N$ dimensional matrix

$$k = \begin{bmatrix} -i\sigma_y & & & \\ & 0 & & \\ & & 0 & \\ & & & -i\sigma_y \end{bmatrix} = \begin{bmatrix} \sigma & & & \\ & 0 & & \\ & & 0 & \\ & & & \sigma \end{bmatrix}, \quad (4.5)$$

where σ is the 2×2 matrix

$$\sigma = -i\sigma_y = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}. \quad (4.6)$$

The matrices K and k satisfy the relations

$$KK^T = I \quad (4.7a)$$

$$kk^T = 1, \quad (4.7b)$$

where I and 1 denote the $4N$ and $2N$ -dimensional unit matrix, respectively.

Equation (4.3) has the consequence that M has the structure

$$M = \begin{bmatrix} \alpha & \beta \\ k\beta^* k^T & k\alpha^* k^T \end{bmatrix} = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}, \quad (4.8)$$

each block being $2N \times 2N$. Equation (4.8) is the extension of (2.1) for particles with spin $1/2$.

Flux conservation is expressed again as in equations (1.9), where each matrix is now $4N \times 4N$. The consequence for α, β (the parallel of Eqs. (2.2)-(2.5)) is now

$$\alpha\alpha^\dagger - \beta\beta^\dagger = 1 \quad (4.9)$$

$$\alpha k\beta^T = \beta k\alpha^T \quad (4.10)$$

or

$$\alpha^\dagger \alpha - k\beta^T \beta^* k^T = 1 \quad (4.11)$$

$$\alpha^\dagger \beta = k\beta^T \alpha^* k^T \quad (4.12)$$

Let $n = 2N$; α, β in (4.8) are then $n \times n$ complex matrices, with a total of $4n^2$ parameters. Equations (4.9) and (4.10) imply n^2 and $n(n+1)$ real restrictions, respectively, so that the total number ν of independent parameters is

$$\nu = 2n^2 - n = 2N(4N - 1). \quad (4.13)$$

According to reference [2], a unitary and self-dual S matrix with dimensionality D has $D(D-1)/2$ parameters; here $D = 4N$, thus giving the same result (4.13).

We now write α, β in their polar representation, just as in (2.6), (2.7); i.e.

$$\alpha = u\ell v \quad (4.14)$$

$$\beta = u' \ell' v', \quad (4.15)$$

u, v, u', v' being $2N \times 2N$ unitary matrices and ℓ, ℓ' , diagonal, real and positive $2N \times 2N$ matrices.

Just as in section 2, suppose u, ℓ, v given. We ask for the most general u', ℓ' ,

v' that satisfy (4.9)-(4.12) (it will turn out that ℓ itself cannot be completely arbitrary). Substituting (4.14), (4.15) in (4.9)-(4.12) we have

$$u\ell^2 u^\dagger - u' \ell'^2 u'^\dagger = 1 \quad (4.16)$$

$$u\ell (vkv'^T) \ell' u'^T = u' \ell' (v' kv^T) \ell u^T \quad (4.17)$$

$$v^\dagger \ell^2 v - (kv'^T) \ell'^2 (v'^* k^T) = 1 \quad (4.18)$$

$$v^\dagger \ell (u^\dagger u') \ell' v' = (kv'^T) \ell' u'^T u^* \ell (v'^* k^T). \quad (4.19)$$

As before, we first construct a particular solution. We try

$$u' = uk, \quad v' = v^* k^T, \quad (4.20)$$

which, substituted in (4.16)-(4.19), give

$$\ell^2 - k\ell'^2 k^T = 1 \quad (4.21)$$

$$k(\ell\ell') k^T = (\ell\ell') \quad (4.22)$$

$$\ell^2 - \ell'^2 = 1 \quad (4.23)$$

$$\ell k\ell' = \ell' k\ell. \quad (4.24)$$

Consider the $2N \times 2N$ diagonal matrix μ

$$\mu = \begin{pmatrix} \mu_1 & & & \\ & 0 & & \\ & & \ddots & \\ & 0 & & \mu_N \end{pmatrix}, \quad \text{with } \mu_i = \begin{pmatrix} \mu_{i+} & 0 \\ 0 & \mu_{i-} \end{pmatrix} \quad (4.25)$$

being 2×2 ; notice that

$$k\mu k^T = \begin{pmatrix} \sigma\mu_1 \sigma^T & & & \\ & 0 & & \\ & & \ddots & \\ & 0 & & \sigma\mu_N \sigma^T \end{pmatrix}, \quad \text{with } \sigma\mu_i \sigma^T = \begin{pmatrix} \mu_{i-} & 0 \\ 0 & \mu_{i+} \end{pmatrix}, \quad (4.26)$$

and

$$\mu k\mu' = \begin{pmatrix} \mu_1 \sigma\mu'_1 & & & \\ & 0 & & \\ & & \ddots & \\ & 0 & & \mu_N \sigma\mu'_N \end{pmatrix}$$

with

$$\mu_i \sigma\mu'_i = \begin{pmatrix} 0 & -\mu_{i+} \mu'_{i-} \\ \mu_{i-} \mu'_{i+} & 0 \end{pmatrix}. \quad (4.27)$$

Using (4.25)-(4.27) in (4.21)-(4.24) we have

$$\ell_{i+}^2 - \ell_{i-}^2 = 1, \quad \ell_{i-}^2 - \ell_{i+}^2 = 1 \quad (4.28)$$

$$\ell_{i+} \ell'_{i+} = \ell_{i-} \ell'_{i-} \quad (4.29)$$

$$\ell_{i+}^2 - \ell_{i+}'^2 = 1, \quad \ell_{i-}^2 - \ell_{i-}'^2 = 1 \tag{4.30}$$

$$\ell_{i+} \ell_{i-}' = \ell_{i+}' \ell_{i-}, \tag{4.31}$$

which imply

$$\ell_{i+} \ell_{i-}, \quad \ell_{i+}' = \ell_{i-}' ; \tag{4.32}$$

ℓ, ℓ' must be of the form

$$\ell = \begin{bmatrix} \ell_1 & & & \\ & \ell_1 & 0 & \\ & 0 & \ell_N & \\ & & & \ell_N \end{bmatrix} \equiv \sqrt{1 + \lambda} \tag{4.33}$$

$$\ell' = \begin{bmatrix} \ell_1' & & & \\ & \ell_1' & 0 & \\ & 0 & \ell_N' & \\ & & & \ell_N' \end{bmatrix} = \sqrt{\lambda} ; \tag{4.34}$$

i.e., the ℓ_a, ℓ_b' must be *degenerate in pairs*.

Our particular solution is thus

$$u' = uk, \quad v' = v * k^T, \quad \ell = \sqrt{1 + \lambda}, \quad \ell' = \sqrt{\lambda}, \tag{4.35}$$

so that $\alpha, \beta, \gamma, \delta$ of (4.8) are given by

$$\alpha = u \sqrt{1 + \lambda} v, \quad \beta = u \sqrt{\lambda} (kv * k^T) \tag{4.36a, b}$$

$$\gamma = (ku * k^T) \sqrt{\lambda} v, \quad \delta = (ku * k^T) \sqrt{1 + \lambda} (kv * k^T) \tag{4.36c, d}$$

and the $4N \times 4N$ transfer matrix M by

$$M = \begin{bmatrix} u & 0 \\ 0 & ku * k^T \end{bmatrix} \begin{bmatrix} \sqrt{1 + \lambda} & \sqrt{\lambda} \\ \sqrt{\lambda} & \sqrt{1 + \lambda} \end{bmatrix} \begin{bmatrix} v & 0 \\ 0 & kv * k^T \end{bmatrix}. \tag{4.37}$$

Of course we have not proved that *any* transfer matrix can be written, in the symplectic case, as in (4.37). We thus proceed to find the most general solution.

From equation (4.16) we have

$$(u'^{\dagger} u) (\ell^2 - 1) (u^{\dagger} u') = \ell'^2 \tag{4.38}$$

Generally speaking, suppose ℓ has the structure (2.9). For instance, in the particular solution studied above, equation (4.33), the ℓ_a 's are degenerate in pairs and the various ℓ_a 's could also be degenerate. Equations (4.38), (A7) and (A6) then give

$$\ell' = P \sqrt{\ell^2 - 1} P^T \tag{4.39}$$

$$u' = ud_1^{\dagger} P^T, \tag{4.40}$$

where d_1 has the structure (2.11).

From equation (4.18) we have, similarly

$$(v'^* k^T v^\dagger) (\ell^2 - 1) (v k v'^T) = \ell'^2, \quad (4.41)$$

so that the lemma gives

$$v' = P d_2^* v^* k, \quad (4.42)$$

d_2 having again the structure (2.11).

We now substitute (4.39), (4.40) and (4.42) in (4.17) and (4.19), obtaining, in both cases

$$d_2^\dagger d_1^* = -d_1^\dagger d_2^* \equiv a = -a^T, \quad (4.43)$$

a being a unitary, antisymmetric matrix with the block structure (2.11). We now find an important property of a . Let x be the matrix of eigenvectors and ν that of the eigenvalues of a ; i.e.

$$ax = x\nu. \quad (4.44)$$

Using $a^T = -a$ we then find

$$a(x^{-1})^T = -(x^{-1})^T \nu. \quad (4.45)$$

Therefore, if ν_i is an eigenvalue, $-\nu_i$ is, too. If the dimensionality of a were odd, at least one of its eigenvalues would have to vanish, contrary to the fact that all the eigenvalues of a unitary matrix must have unit magnitude. Therefore, a can only have even dimensionality, which is what happens in our case ($2N \times 2N$). Since a has the block structure (2.11), the same conclusion applies to each block. Therefore, all of the n_i of (2.9) and (2.11) must be even. The ℓ_i 's of (2.9) are thus at least degenerate in pairs and the ℓ_i 's, in turn, may be degenerate themselves.

We can now write, $\alpha, \beta, \gamma, \delta$ of (4.8) using (4.14), (4.15), (4.40)-(4.43) and with $\ell = \sqrt{1 + \lambda}$, as

$$\alpha = u \sqrt{1 + \lambda} v \quad \beta = u \sqrt{\lambda} (av^* k^T) \quad (4.46a, b)$$

$$\gamma = (ku^* a^\dagger) \sqrt{\lambda} v \quad \delta = ku^* \sqrt{1 + \lambda} v^* k^T \quad (4.46c, d)$$

Notice that equations (4.36) are the particular case of equations (4.46) when $a = k$. We now find the most general form of a .

Suppose first that all the pairs of λ_a are different. Then the matrix a contains 2×2 blocks a_i (see Eq. (2.11)); i.e.

$$a = \begin{bmatrix} a_1 & & & \\ & & 0 & \\ & & & \\ & 0 & & \\ & & & a_N \end{bmatrix}. \quad (4.47)$$

The most general 2×2 unitary antisymmetric matrix a_i is

$$a_i = \begin{pmatrix} 0 & -e^{i\theta_i} \\ e^{i\theta_i} & 0 \end{pmatrix} = e^{i\theta_i} \sigma, \quad (4.48)$$

σ being defined in (4.6). We can then write a as

$$a = \begin{bmatrix} e^{i\theta_1} I_2 & & & \\ & & 0 & \\ & & & \\ & 0 & & \\ & & & e^{i\theta_N} I_2 \end{bmatrix} \begin{bmatrix} \sigma & & & \\ & & 0 & \\ & & & \\ & 0 & & \\ & & & \sigma \end{bmatrix} \equiv e^{i\theta} k = e^{i\theta/2} k e^{i\theta/2} \quad (4.49)$$

where I_2 is the 2×2 unit matrix. Noting that the matrices $e^{i\theta}$ and λ commute, we can write (4.46) as

$$\alpha = u^{(1)} \sqrt{1 + \lambda} u^{(2)}, \quad \beta = u^{(1)} \sqrt{\lambda} [ku^{(2)*} k^T] \quad (4.50a, b)$$

$$\gamma = [ku^{(1)*} k^T] \sqrt{\lambda} u^{(2)}, \quad \delta = [ku^{(1)*} k^T] \sqrt{1 + \lambda} [ku^{(2)*} k^T] \quad (4.50c, d)$$

where we have defined

$$u^{(1)} = u e^{i\theta/2}, \quad u^{(2)} = e^{-i\theta/2} v. \quad (4.51)$$

Finally, M can be written as

$$M = \begin{bmatrix} u^{(1)} & 0 \\ 0 & ku^{(1)*} k^T \end{bmatrix} \begin{bmatrix} \sqrt{1 + \lambda} & \sqrt{\lambda} \\ \sqrt{\lambda} & \sqrt{1 + \lambda} \end{bmatrix} \begin{bmatrix} u^{(2)} & 0 \\ 0 & ku^{(2)*} k^T \end{bmatrix}, \quad (4.52)$$

which has precisely the form of equation (4.37). We can now assert that in the symplectic case, and when $\lambda_1 \neq \dots \neq \lambda_N$ (each λ_a occurring in a pair), *any transfer matrix M can be written in the form (4.52).*

We now consider the general case, when the various λ_a 's may occur more than once. The matrix a contains blocks a_i with even dimensionality n_i (see Eq. (2.11)). At least a large class of unitary and antisymmetric matrices a can be written as

$$a = w a_0 w^T, \quad (4.53)$$

where w is unitary and a_0 is a particular unitary and antisymmetric matrix. We leave it as a conjecture that any unitary and antisymmetric matrix a can be written in the form (4.53). Let's choose $a_0 = k$, so that

$$a = w k w^T \quad (4.54)$$

Equation (4.49) is a particular case of (4.54).

Introducing (4.54) in (4.46) we obtain

$$\alpha = (uw) \sqrt{1 + \lambda} (w^\dagger v), \quad \beta = (uw) \sqrt{\lambda} [k(w^\dagger v)^* k^T] \quad (4.55a, b)$$

$$\gamma = [k(uw)^* k^T] \sqrt{\lambda} (w^\dagger v), \quad \delta = [k(uw)^* k^T] \sqrt{1 + \lambda} [k(w^\dagger v)^* k^T]. \quad (4.55c, d)$$

Defining

$$uw = u^{(1)}, \quad w^\dagger v = u^{(2)}, \quad (4.56)$$

we recover the form (4.50) and hence (4.52) for the transfer matrix. We have thus proved that *in the symplectic case any transfer matrix M can be written in the form (4.52).*

There only remains to study the uniqueness of the composition (4.52).

We start with the case when all λ_a 's are different.

We first illustrate the situation in the simplest case : $N = 1$. Now $u^{(1)}$, $u^{(2)}$ contribute 4 independent parameters each and λ , being a multiple λ' of the 2×2 unit matrix

$$\lambda = \lambda' I_2, \quad (4.57)$$

contributes 1 parameter. We thus have 9 parameters altogether, whereas (4.13) gives $\nu = 6$. However, from equations (4.50) it is not surprising that the special form (4.57) of λ causes some of the combinations of $u^{(1)}$ and $u^{(2)}$ not be independent. To see this, let us insert (4.57) in (4.50); we have

$$\alpha = \sqrt{1 + \lambda'} u^{(1)} u^{(2)} \quad (4.58a)$$

$$\beta = \sqrt{\lambda'} u^{(1)} (\sigma u^{(2)*} \sigma^T), \quad (4.58b)$$

where σ is defined in (4.6). Now, any 2×2 unitary matrix w can be expressed as

$$w = e^{i\phi} s, \quad (4.59)$$

where ϕ is a real number and s is a unitary unimodular 2×2 matrix, which can be written as

$$s = \begin{bmatrix} e^{i(\alpha + \gamma)} \cos \beta & e^{i(\alpha - \gamma)} \sin \beta \\ -e^{-i(\alpha - \gamma)} \sin \beta & e^{-i(\alpha + \gamma)} \cos \beta \end{bmatrix}. \quad (4.60)$$

We can easily check the property

$$\sigma s^* \sigma^T = s. \quad (4.61)$$

Writing

$$u^{(1)} = e^{i\phi_1} s_1 \quad (4.62a)$$

$$u^{(2)} = e^{i\phi_2} s_2 \quad (4.62b)$$

and applying (4.61) to s_2 , α and β of (4.58) can be expressed as

$$\alpha = \sqrt{1 + \lambda'} e^{i\phi} s \quad (4.63a)$$

$$\beta = \sqrt{\lambda'} e^{i\psi} s, \quad (4.63b)$$

where

$$\begin{aligned} \phi &= \phi_1 + \phi_2 \\ \psi &= \phi_1 - \phi_2 \\ s &= s_1 s_2. \end{aligned} \quad (4.64)$$

In (4.63) we have 6 parameters altogether, which is the right number.

We can also look at the above situation in the following way. Using (4.61) we notice that α , β of (4.58) remain invariant if $u^{(1)}$, $u^{(2)}$ are subject to the transformation

$$u^{(1)} \rightarrow u^{(1)} s, \quad u^{(2)} \rightarrow s^\dagger u^{(2)}, \quad (4.65)$$

where s is a unitary unimodular matrix that contains 3 free parameters. This means that we can choose s belonging to the group $SU(2)$ to eliminate 3 parameters out of the 9 we had at the beginning, and we are thus left with 6 free parameters.

We can generalize the above analysis to $N > 1$, when the λ_i are all different from one another. The matrices $u^{(1)}$, $u^{(2)}$ contribute $(2N)^2$ independent parameters each and λ

contributes N parameters. Since each λ_i is doubly degenerate, we again expect to have less than $8N^2 + N$ effectively independent parameters. Indeed, just as above we can prove that α, β of (4.55) remain invariant if the $2N \times 2N$ matrices $u^{(1)}, u^{(2)}$ are subject to the transformation

$$u^{(1)} \rightarrow u^{(1)} \begin{bmatrix} s_1 & & & \\ & 0 & & \\ & & & \\ & & 0 & \\ & & & s_N \end{bmatrix}, \quad u^{(2)} \rightarrow \begin{bmatrix} s_1^\dagger & & & \\ & 0 & & \\ & & & \\ & & 0 & \\ & & & s_N^\dagger \end{bmatrix} u^{(2)}, \quad (4.66)$$

where s_i ($i = 1, \dots, N$) are 2×2 matrices belonging to the group $SU(2)$, containing 3 parameters each. We are thus left with $(8N^2 + N) - 3N = 8N^2 - 2N$ free parameters, just as in (4.13).

We thus conclude that when $\lambda_1 \neq \dots \neq \lambda_N$ the decomposition (4.52) has the arbitrariness expressed by (4.66).

We now turn to the case when the λ_α 's may be repeated. We subject $u^{(1)}$ and $u^{(2)}$ to the transformations

$$u^{(1)} \rightarrow u^{(1)} s \quad u^{(2)} \rightarrow s^\dagger u^{(2)}, \quad (4.67)$$

where s is a unitary matrix with the structure indicated in (2.11). Since $[\lambda, s] = 0$, α of (4.50) remains invariant under (4.67); β transforms as

$$\beta \rightarrow u^{(1)} \sqrt{\lambda} s (ksk^T)^T (ku^{(2)*} k^T). \quad (4.68)$$

In order that β stays invariant, we require that every $n_i \times n_i$ (n_i , even) block $s^{(i)}$ satisfy

$$k_i s^{(i)} k_i^T = s^{(i)*}, \quad (4.69)$$

where k_i contains $n_i/2$ matrices $\sigma(2 \times 2)$ along the diagonal. Since $s^{(i)}$ are unitary, $\det s^{(i)} = e^{i\theta}$; (4.69) implies $\det s^{(i)} = \text{real}$, so that $\det s^{(i)} = \pm 1$; the $+1$ choice indicates that $s^{(i)}$ must belong to the group $SU(n_i)$. But (4.69) implies further restrictions; indeed, if we break $s^{(i)}$ in 2×2 blocks s_{ij} (4.69) reads

$$\begin{aligned} & \begin{bmatrix} \sigma & & & \\ & 0 & & \\ & & & \\ & & 0 & \\ & & & \sigma \end{bmatrix} \begin{bmatrix} s_{11} & s_{1 \frac{n_i}{2}} \\ \cdot & \cdot \\ s_{\frac{n_i}{2} 1} & s_{\frac{n_i}{2} \frac{n_i}{2}} \end{bmatrix} \times \\ & \times \begin{bmatrix} \sigma & & & \\ & 0 & & \\ & & & \\ & & 0 & \\ & & & \sigma \end{bmatrix}^T = \begin{bmatrix} s_{11}^* & s_{1 \frac{n_i}{2}} \\ \cdot & \cdot \\ s_{\frac{n_i}{2} 1}^* & s_{\frac{n_i}{2} \frac{n_i}{2}} \end{bmatrix} \quad (4.70) \end{aligned}$$

so that

$$\sigma s_{ij} \sigma^T = s_{ij}^*, \quad (4.71)$$

implying that the 2×2 block s_{ij} must have the structure

$$s_{ij} = \begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix}. \quad (4.72)$$

We thus have a particular subgroup of $SU(n_i)$.

The conclusion is that in the general case in which the λ_i may be repeated, the decomposition (4.52) has the arbitrariness expressed by (4.67).

Appendix.

We prove the following lemma.

Let μ be an $N \times N$ diagonal matrix, in general with degeneracy, i.e. with the structure

$$\nu = \begin{bmatrix} \mu_1 I_{n_1} & & & \\ & 0 & & \\ & & 0 & \\ & & & \mu_k I_{n_k} \end{bmatrix}, \quad (A1)$$

where μ_i are real numbers and I_{n_i} is the $n_i \times n_i$ unit matrix, with $\sum_{i=1}^k n_i = N$.

Let w be a unitary matrix and suppose that

$$w\mu w^+ = \mu' \quad (A2)$$

is again *diagonal*. Since the eigenvalues of a Hermitean matrix are unique, the diagonal elements of μ' can differ from μ_1, \dots, μ_k only by a permutation. Call P the permutation matrix that takes μ into μ' ; i.e.

$$\mu' = P\mu P^T \quad (A3)$$

Substitute (A3) in (A2)

$$(P^T w) \mu (P^T w)^+ = \mu. \quad (A4)$$

Then the unitary matrix $P^T w$ can only be of the form (2.11); i.e.

$$P^T w = d \quad (A5)$$

or

$$w = Pd. \quad (A6)$$

Notice incidentally that the same matrix P that takes μ into μ' (Eq. (A3)), takes $\sqrt{\mu}$ into $\sqrt{\mu'}$; i.e.

$$\sqrt{\mu'} = P \sqrt{\mu} P^T \quad (A7)$$

References

- [1] WEGNER F., *Phys. Rep.* **67** (1980) 15.
- [2] DYSON F. J., *J. Math. Phys.* **3** (1962) 140.
- [3] PICHARD J. L., SANQUER M., SLEVIN K., DEBRAY P., *Phys. Rev. Lett.* **65** (1990) 1812.
- [4] STONE A. D., MELLO P. A., MUTTALIB K. A. and PICHARD J. L., to appear in « Quantum Effects in small disordered Systems », B. L. Altshuler, P. A. Lee and R. A. Webb Eds. (Elsevier, Amsterdam).
- [5] PICHARD J. L. and SANQUER M., *Physica A* **167** (1990) 66.
- [6] PICHARD J. L., Quantum coherence in mesoscopic systems, B. Kramer Ed. Nato Advanced Studies Institute Series (Plenum, New-York) to appear.
- [7] DOROKHOV O. N., *Solid State Commun.* **44** (1982) 915 ; **46** (1983) 605 ; **51** (1984) 381.
- [8] MELLO P. A., PEREYRA P. and KUMAR N., *Ann. Phys. NY* **181** (1988) 290.
- [9] MELLO P. A. and SHAPIRO B., *Phys. Rev. B* **37** (1988) 5860.
- [10] MELLO P. A., *Phys. Rev. Lett.* **60** (1988) 1089.
- [11] MELLO P. A., AKKERMANS E. and SHAPIRO B., *Phys. Rev. Lett.* **61** (1988) 459.
- [12] MELLO P. A. and STONE A. D., *Phys. Rev. B*, submitted.
- [13] PICHARD J. L. and ANDRÉ G., *Europhys. Lett.* **2** (1986) 477.
- [14] MUTTALIB K. A., PICHARD J. L. and STONE A. D., *Phys. Rev. Lett.* **59** (1987) 2475.
- [15] ZANON N. and PICHARD J. L., *J. Phys. France* **49** (1988) 907.
- [16] BARGMANN V., *Ann. Math.* **48** (1947) 568.
- [17] DYSON F. J., *J. Math. Phys.* **3** (1962) 1191.
- [18] HUA L. K., Harmonic Analysis of Functions of Several Complex Variables in the Classical Domains (L. Ebner and A. Korányi, tr.) Amer. Math. Soc., Providence, R.I., 1963.