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Improper double groups and the bases for the representations of O(3)

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Abstract. Improper double point groups can be defined under two alternative multiplication rules in which the square of the inversion is identified with the identity and with a turn by 2π respectively, although the first rule is the standard one. It is shown that the second multiplication rule can be transformed away into the first one but that, in this process, transformation rules of spinors for $j=\frac{1}{2}$ are obtained which differ from the standard ones, thus solving the following problem. In the standard method, spinors for $j=\frac{1}{2}$ are defined as gerade (even with respect to inversion) and thus their tensor products are incapable of generating a complete set of irreducible bases of O(3), the ungerade harmonics for $j=1$ having to be postulated outside the tensor hierarchy. It is shown that in the new scheme, once the standard multiplication rule for the inversion is defined, spinors for $j=\frac{1}{2}$ appear which are ungerade as well as gerade and thus their tensor products span a complete set of bases of O(3). Comparison is made with the treatment of this problem by projective representations.

1. Introduction

It is well known that a complete set of irreducible bases of SO(3) can be obtained from the tensor products of the spinor basis for $j=\frac{1}{2}$, of components $u_{1/2}^{1/2}$, $u_{-1/2}^{1/2}$, which we shall write as μ_1, μ_2 respectively. We write the *row vector* basis as $\langle\mu_1\mu_2|$ and then, if $g\in \mathrm{SO}(3)$ is parametrised by the Cayley-Klein parameters a, b (see, e.g., Altmann 1986, p 117), the representation of SO(3) is given by

$$g\langle\mu_1\mu_2| = \langle\mu_1\mu_2|\begin{bmatrix} a & b \\ -b^* & a^* \end{bmatrix}. \tag{1.1}$$

We shall be concerned with the improper rotation group O(3), which is written as follows:

$$\mathrm{O}(3)=\mathrm{SO}(3)\otimes C_i,\ C_i=E\oplus \mathbf{i} \tag{1.2}$$

where $\mathbf{i}$ is the inversion. In dealing with O(3), therefore, an expression must be given for the transformation of a spinor under the inversion and it is traditional to use a rule that goes back to Pauli (see, e.g., Altmann 1986, p 108):

$$\mathbf{i}\langle\mu_1\mu_2| = \langle\mu_1\mu_2|\begin{bmatrix} 1 & \\ & 1 \end{bmatrix}. \tag{1.3}$$

This rule, which for convenience we shall call the *Pauli rule*, is standard and must be respected in any treatment of the rotation group. (Although an alternative, called the

Cartan rule, will be presented later in § 3, it must be made clear now that its use is provisional as a step towards recovering equation (1.3) from a different point of view.) The Pauli rule, however, as hitherto used, entails two problems in dealing with the bases of O(3). First, we know that C_i in (1.2) must have two irreducible representations, A_g and A_u, which are gerade (even with respect to inversion) and ungerade (odd) respectively. It is clear that the basis in (1.3), on reduction, will provide a basis for A_g only and thus that no basis for A_u appears directly for $j=\frac{1}{2}$. The second difficulty is a consequence of the first. When forming the (symmetrised) tensor product of two bases $\langle \mu_1 \mu_2|$ in order to obtain the basis for $j=1$, it is clear from (1.3) that the resulting basis is gerade, whereas the spherical harmonics for $j=1$ are ungerade. In order to form a complete set of irreducible bases of O(3) by tensor products, it is thus necessary to postulate an ungerade basis for $j=1$ from outside the tensor hierarchy. Once this is done, the coupling of this basis $j=1$ (ungerade) with the basis $j=\frac{1}{2}$ (gerade) in equation (1.3) will yield a basis of $j=\frac{3}{2}$ (ungerade) and a basis $j=\frac{1}{2}$ (ungerade), the latter providing in this indirect way the missing basis of C_i. The procedure we have just described is used, e.g., by Koster *et al* (1963) and Pyykkö and Toivonen (1983).

The problem of the bases of C_i is treated in Altmann (1986, p 194) by the projective representation method. In this method two alternative factor systems, called the Pauli and Cartan gauges respectively, can be defined. In order to show that this duality is not an artefact of the projective representation method, the double group approach will be used in this paper and it will be demonstrated that for a given improper point group two alternative double groups can be defined, which we shall call the Pauli and Cartan groups respectively, and which differ in the multiplication rule for **i**. We shall see that, ultimately, the Pauli group is the only one that needs to be used. Consideration of the Cartan group, however, will allow the problems stated in this introduction to be solved. Comparison with the projective representation approach will be made in § 4.

2. The double groups

Consider a point group G of operations $g_1 \equiv E, g_2, \ldots, g_n$. A turn by 2π is the identity E for bases of integral j but it multiplies half-integral bases by a phase factor -1, and it is then realised as a new operator $\tilde{E}$, so as to make this behaviour of half-integral bases explicit. $\tilde{E}$ commutes with all $g \in G$ and, on writing $\tilde{E}g$ or $g\tilde{E}$ as $\tilde{g}$ the double group $\tilde{G}$ of G is defined as

$$G = g_1, g_2, \ldots, g_n, \tilde{g}_1, \tilde{g}_2, \ldots, \tilde{g}_n. \tag{2.1}$$

Improper point groups are of two types (see, e.g., Altmann 1977, p 272). The direct product of any point group H with C_i gives an improper point group which contains the inversion:

$$G = H \otimes C_i. \tag{2.2}$$

Improper point groups without the inversion are obtained by first expressing any proper point group G' in cosets of a halving subgroup H (whose order is one half the order of G). Then an improper group G without inversion is written by the following prescription:

$$G' = H \oplus g'H \qquad g' \in G' \qquad g' \notin H \Rightarrow G = H \oplus \mathbf{i}g'H. \tag{2.3}$$

The double groups $\tilde{G}$ corresponding to G in (2.2) or (2.3) are obtained by doubling E into the pair E, $\tilde{E}$, i.e. by substituting $\tilde{H}$ for H in either case:

$$\tilde{G} = \tilde{H} \otimes C_i \qquad G = \tilde{H} \oplus \mathbf{i}g'\tilde{H}. \tag{2.4}$$

The double group O(3) follows at once from (1.2):

$$\tilde{\mathrm{O}}(3) = \widetilde{\mathrm{SO}}(3) \otimes C_i. \tag{2.5}$$

Defining the multiplication rules unambiguously even for a proper double group is not trivial (see Altmann 1986). It is sufficient for our purposes here, however, to draw attention to an important ambiguity in the multiplication rules of $\tilde{\mathrm{O}}(3)$ or of any of its sub-groups (2.4). Whereas, in the single group G, $\mathbf{i}^2$ must be the identity E it can be in $\tilde{G}$ either the identity E or its realisation as a turn by 2π, $\tilde{E}$:

$$\mathbf{i}^2 = E \tag{2.6}$$

$$\mathbf{i}^2 = \tilde{E} \tag{2.7}$$

a point which is noted by Berestetskii *et al* (1971, p 58). It will be convenient to call (2.6) and (2.7) the Pauli and the Cartan multiplication rules. It should be clear that, with these rules, any improper point group G yields two realisations of two *distinct* abstract groups. Thus, each double group $\tilde{G}$ can be understood as either $\tilde{G}_{\mathrm{p}}$ or $\tilde{G}_{\mathrm{c}}$, the Pauli and Cartan double groups respectively. We shall presently show, however, that these two groups lead to the same observables in physical applications.

If, given an operator g, we denote with $\hat{g}$ its matrix representative, we know that, in all representations,

$$\hat{E} = \mathbf{1} \qquad \hat{\tilde{E}} = -\mathbf{1} \tag{2.8}$$

where $\mathbf{1}$ is the unit matrix of the same dimension as that of the representation in question. If we introduce (2.8) into (2.6) and (2.7) we immediately obtain:

$$\hat{\mathbf{i}} = \mathbf{1} \qquad \mathbf{i} \in \tilde{G}_{\mathrm{p}} \tag{2.9}$$

$$\hat{\mathbf{i}} = -\mathrm{i}\mathbf{1} \qquad \mathbf{i} \in \tilde{G}_{\mathrm{c}} \tag{2.10}$$

where the minus sign in (2.10) is arbitrary and has been added for later convenience. In order to understand the meaning of the difference between (2.9) and (2.10) we recall that for any operator g and a basis of functions $\phi_1, \phi_2, \ldots, \phi_n$ written as a row vector $\langle \phi_1, \phi_2, \ldots, \phi_n|$, the action of g on the basis is given by

$$g\langle \phi_1\phi_2 \ldots \phi_n| = \langle \phi_1\phi_2 \ldots \phi_n|\hat{g}. \tag{2.11}$$

Thus, the difference between (2.9) and (2.10) is that, in the latter case, the basis is multiplied by $-\mathrm{i}$ for all operations which contain the inversion. This is a phase factor which cannot affect the energy. Also, such a phase factor cannot affect the irreducibility of a representation (because the sum of the moduli squared of the characters remains invariant) or their orthogonality.

It follows from the above that the difference between the Cartan and Pauli double groups is, in principle, trivial. One can easily go from the Cartan to the Pauli group by multiplying the operators which contain the inversion with the factor $+\mathrm{i}$ (see (2.10)). Such a factor will be called a *gauge factor* (see § 4).

It is tempting to conclude from the above that the Cartan double group is of little interest and should be replaced by the simpler Pauli double group, and this is probably the reason not only for the hitherto universal use of the Pauli rule but also for the complete neglect of the Cartan one. We shall see, however, that when the Cartan double group is used as an intermediate step towards the construction (by a change of gauge) of the Pauli double group some useful results appear about the symmetry behaviour of the spinor bases.

3. Behaviour of the spinor basis under inversion

We shall first work within the Pauli double group. If g is a proper rotation of $\tilde{\mathrm{O}}(3)$, its action on the spinor $\langle \mu_1 \mu_2|$ is given by (1.1), whereas for $\mathbf{i}$ (2.9) gives

$$\mathbf{i}\langle \mu_1\mu_2| = \langle \mu_1\mu_2| \begin{bmatrix} 1 & \\ & 1 \end{bmatrix} \qquad \mathbf{i} \in \tilde{\mathrm{O}}(3)_{\mathrm{P}} \tag{3.1}$$

in agreement, of course, with the standard rule (1.3). We want to consider also the complex conjugate spinor $\langle \mu_1^* \mu_2^*|$, the matrices for which are obtained by complex conjugation on (1.1) and (3.1):

$$g\langle \mu_1^*\mu_2^*| = \langle \mu_1^*\mu_2^*| \begin{bmatrix} a^* & b^* \\ -b & a \end{bmatrix} \tag{3.2}$$

$$\mathbf{i}\langle \mu_1^*\mu_2^*| = \langle \mu_1^*\mu_2^*| \begin{bmatrix} 1 & \\ & 1 \end{bmatrix} \qquad \mathbf{i} \in \tilde{\mathrm{O}}(3)_{\mathrm{P}}. \tag{3.3}$$

It is clear that the matrices in (3.2) and (1.1) have the same trace, and that those in (3.1) and (3.3) are identical. Thus, $\langle \mu_1\mu_2|$ and $\langle \mu_1^*\mu_2^*|$ must belong to equivalent representations and it is easy to obtain the transformation of $\langle \mu_1^*\mu_2^*|$ which will make both representations identical:

$$g\langle \mu_2^*, -\mu_1^*| = \langle \mu_2^*, -\mu_1^*| \begin{bmatrix} a & b \\ -b^* & a^* \end{bmatrix} \tag{3.4}$$

$$\mathbf{i}\langle \mu_2^*, -\mu_1^*| = \langle \mu_2^*, -\mu_1^*| \begin{bmatrix} 1 & \\ & 1 \end{bmatrix} \qquad \mathbf{i} \in \tilde{\mathrm{O}}(3)_{\mathrm{P}}. \tag{3.5}$$

It is clear that, in the Pauli double group, except for the trivial rearrangement shown in the last two equations, a spinor and its conjugate span identical representations. This will no longer be the case in the Cartan double group, as we shall now demonstrate.

In the Cartan double group, clearly, (1.1) and (3.4) are still valid for a proper rotation g, whereas from (2.10), (3.1) for $\mathbf{i}$ is replaced by

$$\mathbf{i}\langle \mu_1\mu_2| = \langle \mu_1\mu_2| \begin{bmatrix} -\mathrm{i} & \\ & -\mathrm{i} \end{bmatrix} \qquad \mathbf{i} \in \tilde{\mathrm{O}}(3)_{\mathrm{c}}. \tag{3.6}$$

Correspondingly,

$$\mathbf{i}\langle \mu_2^*, -\mu_1^*| = \langle \mu_2^*, -\mu_1^*| \begin{bmatrix} \mathrm{i} & \\ & \mathrm{i} \end{bmatrix} \qquad \mathbf{i} \in \tilde{\mathrm{O}}(3)_{\mathrm{c}}. \tag{3.7}$$

It is clear that as a difference with the Pauli group a spinor and its conjugate span non-equivalent representations in the Cartan double group. The significance of this result will become apparent when we go over from (3.6) and (3.7) to the Pauli group, the latter being the standard and most practical realisation of the double group. We have seen in § 2 that one passes from the Cartan to the Pauli group by multiplying the improper operations with i. When this is done, (3.6) and (3.7) give, respectively,

$$\mathbf{i}\langle\mu_1\mu_2| = \langle\mu_1\mu_2|\begin{bmatrix}1 & \\ & 1\end{bmatrix} \qquad \mathbf{i}\in\tilde{\mathrm{O}}(3)_{\mathrm{P}} \tag{3.8}$$

$$\mathbf{i}\langle\mu_2^*, -\mu_1^*| = \langle\mu_2^*, -\mu_1^*|\begin{bmatrix}-1 & \\ & -1\end{bmatrix} \qquad \mathbf{i}\in\tilde{\mathrm{O}}(3)_{\mathrm{P}}. \tag{3.9}$$

Equation (3.8) coincides of course with (3.1) (it is for this purpose that the negative sign was chosen in (2.10), and verifies that we have now returned to the Pauli group, in which spinors are gerade. But, whereas in the previous presentation of the Pauli group conjugate spinors were also gerade, (3.9) shows that, even within the Pauli group, conjugate spinors do not span the same representation as spinors but rather that they are ungerade.

4. The bases of O(3)

From (2.5), it is useful to consider first the bases of $C_i \subset \tilde{\mathrm{O}}(3)$. From our first presentation of the Pauli group in (3.1) and (3.3) it is clear that the two operations E and $\mathbf{i}$ of C_i are represented by the matrices $\mathbf{1}_2$ and $\mathbf{1}_2$ respectively, unit matrices of dimension two. On reduction, this representation gives the single representation for which $\hat{E}$ and $\hat{\mathbf{i}}$ are respectively 1 and 1, i.e. the gerade representation A_{g}. It is clear that no ungerade representation can be derived directly from bases with $j=\frac{1}{2}$. In our second presentation of the Pauli group, via the Cartan group, there are two non-equivalent representations of C_i. In the first $\hat{E}=\mathbf{1}_2$, $\hat{\mathbf{i}}=\mathbf{1}_2$, with basis $\langle\mu_1\mu_2|$ (see (3.8)), and in the second $\hat{E}=\mathbf{1}_2$, $\hat{\mathbf{i}}=-\mathbf{1}_2$, with basis $\langle\mu_2^*, -\mu_1^*|$ (see (3.9)). The first representation will reduce into A_{g} as defined before, with basis $u_{1/2}^{1/2}$ (one of the spinor components) and the second will reduce into a representation A_{u} in which $\hat{E}=1$, $\hat{\mathbf{i}}=-1$, clearly ungerade and with basis $(u_{1/2}^{1/2})^*$. We have now found the missing basis of C_i thus solving the first problem discussed in § 1. It is also clear how the second problem therein stated is solved. We now have two bases of $\tilde{\mathrm{O}}(3)$ for $j=\frac{1}{2}$, $\langle\mu_1\mu_2|$ (gerade) and $\langle\mu_2^*, -\mu_1^*|$ (ungerade). On forming the direct product of these two bases we must get an ungerade four-dimensional basis which, from the Clebsch–Gordan rule, must reduce into two bases, one for $j=1$, ungerade, dimension 3 (symmetrised tensor product), and one for $j=0$, ungerade, dimension 1 (antisymmetrised tensor product). The first is the spherical harmonic $j=1$ which hitherto had to be postulated, since it was unobtainable as a tensor product from $j=\frac{1}{2}$ spinors, and the second basis is a pseudoscalar.

In order to discuss the bases of $\tilde{\mathrm{O}}(3)$ we first consider those of $\widetilde{\mathrm{SO}}(3)$, for which purpose $\langle u^{1/2}|$, $\langle u^1|$, etc, will denote the irreducible bases for $j=\frac{1}{2}$, 1, etc, respectively. In $\widetilde{\mathrm{SO}}(3)$, $\langle u^{1/2}|$ and $\langle u^{1/2}|^*$ belong to the same irreducible representation for $j=\frac{1}{2}$, (although they are g and u respectively, but $\mathbf{i}\notin\widetilde{\mathrm{SO}}(3)$). Bases for $j=1$ are obtained from $\langle u^{1/2}|\otimes\langle u^{1/2}|, (g)$; $\langle u^{1/2}|^*\otimes\langle u^{1/2}|^*, (g)$; $\langle u^{1/2}|\otimes\langle u^{1/2}|^*, (u)$, all of which belong to the same representation. On denoting $\langle u^1|_{\mathrm{g}}$, $\langle u^1|_{\mathrm{u}}$ the bases so far defined, the bases for $j=\frac{3}{2}$ are then obtained from

$$\langle u^1|_{\mathrm{g}}\otimes\langle u^{1/2}|, (g) \qquad \langle u^1|_{\mathrm{u}}\otimes\langle u^{1/2}|^*, (g)$$

$$\langle u^1|_{\mathrm{u}}\otimes\langle u^{1/2}|, (u) \qquad \langle u^1|_{\mathrm{g}}\otimes\langle u^{1/2}|^*, (u)$$

all of which belong to the same representation. The same applies for higher values of j. In $\tilde{\mathrm{O}}(3)$, from the relation $\tilde{\mathrm{O}}(3)=\widetilde{\mathrm{SO}}(3)\otimes C_i$, each of the representations of $\widetilde{\mathrm{SO}}(3)$ splits in two, one gerade and the other ungerade, and the bases described above now separate into these two representations, in accordance to their parity. It will be seen that the scheme proposed describes very simply and naturally all the bases of $\tilde{\mathrm{O}}(3)$. The basis $\langle u^1|_g$ corresponds to the basis S_x, S_y, S_z defined in a somewhat arbitrary fashion by Koster *et al* (1963).

5. Discussion

The work which we have done is considerably streamlined on using the projective representation approach as discussed in Altmann (1986). Whereas in an ordinary (vector) representation the product of the matrix representatives of g_i and g_j is the matrix representative of g_ig_j, in a projective representation a *projective factor* appears on the right-hand side, which is a complex number depending on g_i and g_j. It can now be proved (see below) that two different projective factors can be chosen for the product $\mathbf{i}^2$, $+1$, and -1, respectively called the Pauli and Cartan factors. Given a projective representation a so-called *change of gauge* can be effected by multiplying the matrix of each operation g_i by a stated complex number. This will result in a new factor system. If the matrices for $\mathbf{i}$ are multiplied by i, the Cartan factor system or Cartan gauge changes into the Pauli gauge, which parallels precisely what we have done in the double group and explains the terminology adopted.

Altmann (1986) gives various reasons for the use of the Cartan projective factor -1 for $\mathbf{i}^2$, but important support for its use derives from the use of the Clifford algebra. In the Clifford algebra $\mathscr{C}_3$ with unit elements e_1, e_2, e_3 such that

$$e_ie_j+e_je_i=2\delta_{ij} \tag{5.1}$$

it is shown that the product $e_1e_2e_3$ maps into the inversion $\mathbf{i}$ (see Altmann 1986, p 222). It is now simple to prove from (5.1) that

$$e_1e_2e_3e_1e_2e_3=-1 \tag{5.2}$$

thus verifying the Cartan factor.

The significance of a spinor transformation such as (1.3) must be discussed. Because spinor components are homogeneous coordinates in a projective plane, it is their ratio $\mu_1:\mu_2$ which is significant rather than their individual values. That is, μ_1 and μ_2 can each be multiplied by an arbitrary factor without changing the physical meaning of the spinor. Because the spinor invariant $\mu_1^*\mu_1+\mu_2^*\mu_2$ must be preserved, this factor ω must be a phase factor. This means that the transformation matrix $\mathbf{1}$ in (1.3) should be written in a more general form as $\omega\mathbf{1}$. Because the representative of $\mathbf{i}^2$ must be ± 1 it follows that ω can be ± 1 or $\pm$i. Thus, the transformation rule (1.3) is quite conventional and it could be changed (re-gauged) into one with any of the matrices in (3.6)–(3.9). The choice of the transformation rules under the inversion for the spinor and its complex conjugate is, therefore, within these limits, quite arbitrary. What we have done is to show how this choice can be done in a consistent and useful way.

Finally, a short reference to relativistic spinors may be useful. It is well known that in relativity a distinction must always be made between a spinor and its complex conjugate, the latter components being conventionally denoted with dots or primes (see Berestetskii *et al* 1971, Woodhouse 1980). The problem of space inversion in this case has been considered by Niederer and O'Raifeartaigh (1974) and Staruszkiewicz (1976). The first-mentioned authors, in particular, prove that relativistic spinors separate out in two types which have the same transformation properties under SU(2), but which transform differently under inversion.

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