REPRESENTATIONS OF THE MAGNETIC SYMMETRY GROUPS*

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RESUMEN

Para estudiar los grupos de simetría de una red cristalográfica en presencia de un campo magnético deben considerarse las representaciones proyectivas de dichos grupos, debido al cambio de fase que sufren las funciones de onda y que proviene de las transformaciones de norma que acompañan a las simetrías geométricas. Estas representaciones proyectivas son representaciones ordinarias de un grupo que es isomórfico a los grupos generalizados de Dirac. Las representaciones irreducibles y las funciones adaptadas a la simetría de dichos grupos se pueden obtener mediante técnicas que resultan del método de representaciones inducidas para los grupos que se pueden exhibir como productos semi-directos.

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SUMMARY

In studying the symmetry groups of a crystal lattice in the presence of a magnetic field, the projective representations of these groups must be considered, because of the phase change in the wave functions which is due to the gauge transformations which accompany the geometric symmetries. These projective representations are ordinary representations of a group which is isomorphic to the generalized Dirac groups. The irreducible representatioos of the symmetry-adapted functions of these groups can be obtained by means of techniques arising from the method of induced representations for those groups which can be exhibited as semi-direct products.

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If we transform the vector potential of a magnetic field in such a way that

$$A' = A + \nabla f(x, y, z) \tag{1}$$

the wave functions of the stationary states of a particle in such a magnetic field are not the same as for the original Hamiltonian, but differ with respect to a phase factor[1]; that is

$$\psi \rightarrow \psi e^{i\varepsilon f(x, y, z)}; \quad \varepsilon = -e/\hbar c . \tag{2}$$

Thus, while such a transformation alters the Hamiltonian $H = (p - e/cA)^2 + V(x, y, z)$ and thus is not a symmetry of the problem, it nevertheless does not affect any observable quantities which depend upon the absolute value of the wave function. A symmetry operation for such a Hamiltonian thus consists of the gauge transformation (1) together with the corresponding phase change (2).

Also we know[2] that coordinate transformations such as translations, rotations or reflections, or combinations of these, induce changes in the vector potentials that in some cases can be gauge transformations of the form (1), so that these transformations are not strictly symmetry operations even in the presence of a symmetric potential, although it is possible to compensate their effect with an appropriate gauge transformation.

Such transformations change the wave function in such a way that

$$\psi_\lambda(r') = e^{i\varepsilon f(xyz)} \sum C^f_{\lambda\lambda'} \psi_\lambda(r) \tag{3}$$

where r' is the transformed position vector, $\Delta A = \nabla f(x, y, z)$ is the gauge transformation induced by the transformation of coordinates, and $C^f_{\lambda\lambda'}$ is the matrix that represents the mixing of states caused by the transformation.

The most general symmetry in the case of a uniform magnetic field consists of a general translation together with an arbitrary rotation about the field direction and a possible reflection perpendicular to the field axis.

To prove this let us remember that Harper[3] proved that any translation is a symmetry and that the corresponding gauge transformation is

$$\Delta A_t = \nabla [A(t) \cdot r] \tag{4}$$

and let us consider that the magnetic field is given

$$H = - \begin{bmatrix} \alpha \\ \beta \\ \gamma \end{bmatrix}$$

in an orthogonal coordinate system. Then we can take the vector potential as

$$A(r) = \begin{bmatrix} \alpha y \\ \beta z \\ \gamma x \end{bmatrix} \tag{5}$$

that is

$$A(r) = Mr, \quad M = \begin{bmatrix} 0 & \alpha & 0 \\ 0 & 0 & \beta \\ \gamma & 0 & 0 \end{bmatrix} \tag{6}$$

Now if R is the matrix that represents a transformation of coordinates formed by a rotation together with a reflection, the vector potential that appears after such a transformation is

$$A' = R^{-1} A(Rr) = R^{-1} M R r \tag{7}$$

where R^{-1} has to appear due to the adjustment of the local system of coordinates. Then,

$$\Delta A = A' - A = [R^{-1} M R - M] r \tag{8}$$

Now, the integrability conditions for ΔA, that is the conditions which must be satisfied so that we can write (8) in the form of (1), are

$$[R^{-1} M R - M]^T = R^{-1} M R - M \tag{9}$$

or in other words that the matrix coefficient defining ΔA is symmetric. Observing that for rotations and reflections,

$$R^{-1} = R^T,$$

we can write (9) in the form

$$R^{-1}(M^T - M) R - (M^T - M) = 0 \tag{9'}$$

Now breaking M into its symmetric and antisymmetric parts, $M = M^s + M^a$, (9') reduces to

$$R^{-1} M^a R - M^a = 0,$$

or

$$M^a R = R M^a \tag{10}$$

So we see that the integrability condition is that the antisymmetric part of the vector potential matrix commutes with the transformation matrix, which means that they have a common set of eigenvectors. The real eigenvector of M^a,

$$M^a = \frac{1}{2} \begin{bmatrix} 0 & \alpha - \gamma \\ -\alpha & 0 & \beta \\ \gamma - \beta & 0 \end{bmatrix}$$

is

$$\begin{bmatrix} \beta \\ \gamma \\ \alpha \end{bmatrix}$$

which is the direction of the magnetic field. Thus the integrability condition is that the axis of the field should be parallel to the axis of the operation.

Now, introducing the integrability condition (10) in (8), we see that

$$\nabla A = R^{-1} M^s R - M^s \tag{11}$$

and hence that

$$\Delta A = \nabla \phi$$

if

$$\phi = \frac{1}{2} Kr \cdot r$$

where

$$K = R^{-1} M^s R - M^s$$

$$M^s = \frac{1}{2} (M + M^t)$$

$$M^s = \frac{1}{2} \begin{vmatrix} 0 & \alpha & \gamma \\ \alpha & 0 & \beta \\ \gamma & \beta & 0 \end{vmatrix}$$

and as a consequence we can write:

1) For a translation the wave function transforms as

$$\psi_\lambda (r + t) = e^{i\varepsilon Mt \cdot r} \sum_{\lambda'} C^t_{\lambda\lambda} \psi_{\lambda'} (r) \tag{12}$$

2) For a rotation (reflection) the wave function transforms as

$$\psi_\lambda (Rr) = e^{i\varepsilon \frac{1}{2} Kr \cdot r} \sum_{\lambda'} C^R_{\lambda\lambda'} \psi_{\lambda'} (r) \tag{13}$$

Now, under the same conditions, let us consider a rotation or reflection followed by a translation. By the same method we find that

$$\Delta A = [R^{-1} MR - M] r + R^{-1} Mt$$

In this case the integrability condition is obviously the same, namely that the axis of the rotation or reflection is parallel to the axis of the field without any restriction on the translations. Hence

$$\Delta A = \nabla [\{ \frac{1}{2} Kr \cdot r + R^{-1} Mt \} \cdot r] \tag{14}$$

and in this case the wave function transforms as

$$\psi_\lambda (Rr + t) = e^{i\varepsilon (\frac{1}{2} Kr \cdot + R^{-1} Mt) \cdot r} \sum C_{\lambda\lambda'} \psi_{\lambda'} (r)$$

Now let us consider the group of translations $\{t\}$. We see that the matrices

$$D(t) = e^{i\varepsilon Mt \cdot r} | C^t | \tag{16}$$

form a representation of this group; furthermore because

$$D(t_1)\,D(t_2) = e^{i\varepsilon[Mt_1\cdot(r+t_2)+Mt_2\cdot r]}\,C^{t_1}_{\lambda\lambda'}\,C^{t_2}_{\lambda\lambda'}$$

$$D(t_1+t_2) = e^{i\varepsilon M(t_1+t_2)\cdot r}\,C^{t_1+t_2}_{\lambda\lambda'} \tag{17}$$

we can write

$$D(t_1)\,D(t_2) = e^{-i\varepsilon Mt_2\cdot t_1}\,D(t_1+t_2) \tag{18}$$

observing that

$$C^{t_1+t_2} = e^{i\varepsilon Mt_1\cdot t_2}\,C^{t_2}\,C^{t_1}\ .$$

so that this representation is projective. Moreover, using (18) we can see that

$$D(t_1)\,D(t_2) = e^{i\varepsilon[Mt_2\cdot t_1 - Mt_1\cdot t_2]}\,D(t_2)\,D(t_1) \tag{19}$$

so that the representation is not commutative. The commutation rule (19) also tells us that, as we shall see in detail later, we are dealing with an induced representation in the sense of reference 4.

Now let us turn our attention to the group of transformations whose matrices obey the integrability condition (10). This group is formed by rotations about the axis of the field and reflections perpendicular to the field axis.

We see that the matrices

$$D(R) = e^{i\varepsilon\frac{1}{2}Kr\cdot r}\,|C^{R}_{\lambda\lambda'}| \tag{20}$$

form a representation of this group, and furthermore because

$$D(R_1)\, D(R_2) = e^{i\varepsilon \frac{1}{2}[K_1 R_2 r \cdot R_2 r + K_2 r \cdot r]} \, | C^{R_1}_{\lambda\lambda'} | \, | C^{R_2}_{\lambda\lambda'} |$$

$$D(R_1 R_2) = e^{i\varepsilon \frac{1}{2}[K_{12} r \cdot r]} \, | C^{R_1 R_2}_{\lambda\lambda'} |$$

we can write

$$D(R_1 R_2) = e^{i\varepsilon \frac{1}{2}[K_1 R_2 r \cdot R_2 r - K_1 r \cdot r]} D(R_1)\, D(R_2) \qquad (21)$$

observing that

$$C^{R_1 R_2} = C^{R_1} C^{R_2} \; .$$

We could then rewrite (21) as

$$D(R_1 R_2) = e^{i\varepsilon \frac{1}{2}[R_2 \hat{K}_1 r \cdot R_2 r - K_1 r \cdot r]} D(R_1)\, D(R_2) \qquad (22)$$

where $\hat{K}_1 = R_2^{-1} K_1 R_2$.

Thus it is seen that this representation is also projective. We moreover see that

$$D(R_1)\, D(R_2) =$$

$$\exp \left[i\varepsilon \frac{1}{2} (R_1 \hat{K}_2 r \cdot R_1 r - R_2 \hat{K}_2 r \cdot R_2 r + K_1 r \cdot r - K_2 r \cdot r) \right] D(R_2)\, D(R_1) \qquad (23)$$

so that this representation is not commutative, even though the rotations are about the same axis, or possible reflections are compatible with them. On the other hand, in the same manner as for the translation group, as outlined in reference 4, this rule permits one to deduce that the representations are induced.

Let us now turn our attention toward the structure of the general symmetry group. If we apply a rotation or reflection to a vector r, followed by a translation, the resulting vector is

$$r' = R_1 r + t_1 .$$

If we apply to this vector r' another rotation or reflection and yet another translation we obtain

$$r'' = R_2 r' + t_2 = R_2 R_1 r + R_2 t_1 + t_2$$

which is the same as a rotation $R_2 R_1$ followed by the translation $R_2 t_1 + t_2 = \hat{t}_1$.

In view of this, we notice that the group is a semidirect product of the group of translations and the group of rotations-reflections, considering the latter group as an autmorphism group for the first.

Returning to (15), we see that

$$D(R_2 t_2 , R_1 t_1) =$$

$$\exp(i\varepsilon [\frac{1}{2} K_2 (R_1 r + t_1) + R_2^{-1} M t_2] (R_1 r + t_1) - \frac{1}{2} (K_2 r + R_2^{-1} M t_2) \cdot r]$$

$$\times D(R_2 t_2) D(R_1 t_1)$$

which shows that the representation of the entire group is also projective.

Since the semidirect product group as a whole is non-commutative one cannot immediately deduce a commutation rule for the elements of the type which defines a "Dirac group" (ref. 4), but bearing in mind that we have a projective representation,

$$D(a) D(b) = \lambda(a, b) D(ab)$$

we can indeed find a rule of the form

$$D(a)\,D(b) = \frac{\lambda(a,b)}{\lambda(b,b^{-1}ab)}\,D(b)\,D(b^{-1}ab),$$

which is still sufficiently of the form of an exchange rule that it is possible to determine the representation as an induced representation. In our present case this multiplier turns out to be a_1/a_2, with

$$a_1 = \exp(i\varepsilon[\tfrac{1}{2}K_1(R_2r + t_2) + R_1^{-1}Mt_1)\cdot(R_2r + \hat{t}_2) - \tfrac{1}{2}(K_1r + R_1^{-1}Mt_1)\cdot r])$$

$$a_2 = \exp(i\varepsilon[\tfrac{1}{2}K_2(R_1r + \hat{t}_1) + R_2^{-1}Mt_2)\cdot(R_1r + \hat{t}_1) - \tfrac{1}{2}(K_1r + R_1^{-1}M\hat{t}_1)\cdot r]) \qquad (25)$$

In summary, we have laid the groundwork to show that when the change of phase due to gauge transformation is taken into account, one obtains a projective representation of an appropriate two-dimensional lattice group as the symmetry group of a particle moving in a periodic potential in the presence of a uniform magnetic field.

Given such a projective representation, one can proceed to determine the possible irreducible representations to which it might correspond by deducing appropriate exchange relations and applying the theory of Dirac groups.

REFERENCES

1. L.D. Landau and F.M. Lifshitz, QUANTUM MECHANICS, Pergamon Press, 1962 p. 472.
2. V.A. Dulock Jr., Thesis, University of Florida, 1964, p. 77-81.
3. P.G. Harper, Proc Roy Soc **A68** 874 (1955).
4. A. Deepak, B.S. Thomas, V.A. Dulock Jr., & H.V. McIntosh, preprint #58, Quantum Theory Project, University of Florida, 1964.