Spin-Orbit Coupling in Band Theory—Character Tables for Some "Double" Space Groups

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To take account of the electron spin in band theory, a method is outlined which allows us to construct character tables for the double space groups of the simple, face-centered, and body-centered cubic, diamond, and hexagonal close packed lattices. The effects of time reversal are also considered. Particular attention is given to the splitting of otherwise degenerate bands by the spin-orbit coupling.

THE symmetry of crystal lattices has important effects on the band theory of electron energy states. Bouckaert, Smoluchowski, and Wigner[1] have considered the group theoretical properties of these symmetries and constructed character tables of the irreducible representations for some simple lattices while Herring[2] has extended this to more complicated lattices.

It has recently become evident from measurements of magnetic properties like paramagnetic resonance,[3,4] that the coupling of the electron spin to the orbital motion has important effects. Moreover this spin-orbit coupling can introduce changes in energy of the order of the atomic spin-orbit coupling constant (0.1 ev or more in crystals of heavy atoms) and may therefore greatly change the details of the band form. This may be very important when we are considering properties of electrons with a kinetic energy which is only of the order of this spin-orbit coupling energy, such as occurs for example in impurity semiconductors.[5]

It therefore seemed of some interest to consider the effect of spin-orbit coupling on the symmetry properties of the bands. In this paper we outline a method and use it to construct character tables for a number of interesting space groups which are applicable when the spin is included. Bethe[6] and Opechowski[7] have shown in the case of point groups that this may be achieved by constructing the "double" group and their methods may be readily extended to space groups. Extra degeneracies are also caused by time-reversal symmetry and it is found that the general considerations of Wigner,[8] which were used for ordinary space groups by Herring,[9] can be readily applied to the dosuble group. The most significant effects of spin-orbit coupling arise when it removes degeneracies in the bands, and this effect can be readily seen by inspection of the character tables.

GENERAL THEORY

The Schrödinger equation of an electron in a crystal when spin-orbit coupling is included is

$$\left[-\frac{\hbar^2\nabla^2}{2m}+V+\frac{\hbar}{4m^2c^2}(\boldsymbol{\nabla} V\times\mathbf{p}\cdot\boldsymbol{\sigma})\right]\psi=\epsilon\psi.$$

The Hamiltonian operator and therefore the state function still have the translation and point symmetry of the lattice. We can therefore still obtain the symmetry properties of ψ by considering the space group of the crystal. This consists of an invariant subgroup of translations and a set of operations which leave the unit cell invariant. In simple lattices like simple cubic (s.c.), face-centered cubic (f.c.c.), and body-centered cubic (b.c.c.), this latter set is an invariant subgroup of the space group and is a point group (a subgroup of the full rotation group) but in more complicated lattices like diamond and hexagonal close packed (h.c.p.), it contains elements which consist of a rotation about a point together with a translation. We shall therefore employ in these cases the notation introduced by Seitz[10] and used by Herring.[2] The operation $[\alpha|a]$ represents a rotation α about the origin followed by a vector translation $\mathbf{a}$. The product of two such elements is given by

$$[\alpha|a][\beta|b]=[\alpha\beta|a+\alpha b].$$

Seitz showed that any irreducible representation can be based on a set of functions of the type $u_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{r}}$ (i.e., on the usual Bloch electron wave functions) each of which represents an element $[\epsilon|t]$ of the translation group by $\exp(-i\mathbf{k}\cdot\mathbf{t})$ (ϵ is used for the unit element of the rotation group throughout the paper). Operating on this basis function with some elements of the unit cell group we shall transform it into a function with wave vector different from $\mathbf{k}$. All wave vectors which can be reached from $\mathbf{k}$ in this way are called the "star" of $\mathbf{k}$.[1] We are interested in energy degeneracies for wave functions with a fixed $\mathbf{k}$. We therefore consider that subgroup G^k of the space group which

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[1] Bouckaert, Smoluchowski, and Wigner, Phys. Rev. **50**, 58 (1936).
[2] C. Herring, J. Franklin Inst. **233**, 525 (1942).
[3] Portis, Kip, Kittel, and Brittain, Phys. Rev. **90**, 988 (1953).
[4] R. J. Elliott, preceding paper, Phys. Rev. **95**, 266 (1954). (See this paper for further references.)
[5] Discussion of the relation of the band forms to measurements of properties like magnetoresistance has been given by C. Herring (private communication).
[6] H. A. Bethe, Ann. Physik **3**, 133 (1929).
[7] W. Opechowski, Physica **7**, 552 (1940).
[8] E. Wigner, Göttingen Nachr. p. 546 (1932).
[9] C. Herring, Phys. Rev. **52**, 361 (1937).
[10] F. Seitz, Ann. Math. **37**, 17 (1936).

contains only those elements which transform a basis into one with the same $\mathbf{k}$. At a general point in the Brillouin zone this will consist only of the translation group, but at a place of high symmetry a subgroup of the unit cell group will also be included. That subgroup T^k of the translation group $(\epsilon|t)$ such that $\exp(i\mathbf{k}\cdot\mathbf{t})=1$ can also be removed since each element is equivalent to the unit element. We are left with a factor group G^k/T^k which can be greatly simplified because it is usually a direct product of an abelian subgroup which consists of most of the translations together with the subgroup which consists of the unit cell element in G^k with possibly a few translations. In simple lattices, s.c., f.c.c., b.c.c., the unit cell elements are rotations and this product is simply that of a subgroup of translations T/T^k and one of rotations G^k/T, but the more complicated conditions apply if there are screw axes or glide planes in the group.

All these considerations hold in exactly the same way when we consider spin except that we now consider double groups. Opechowski shows how to construct these for any group of rotations. He points out that the rotation group δ_3 is isomorphous with the group of 2×2 unitary matrices with determinant $+1$. For any rotation a matrix can be written

$$\begin{pmatrix} \alpha & -\beta^* \\ \beta & \alpha^* \end{pmatrix} \quad |\alpha|^2+|\beta|^2=1,$$

and if we specify the rotation by Euler angles (θ,ϕ,ψ), $\beta=\sin\frac{1}{2}\theta e^{i(\phi-\psi)/2}$ and $\alpha=\cos\frac{1}{2}\theta e^{-i(\phi+\psi)/2}$.[11] This representation of the rotation group is however two valued since the matrix with all the elements changed in sign is also isomorphous with the rotation. This two valuedness is just what is required to include spin, and we therefore work with a group in which each rotation corresponds to two elements which can be represented by these two matrices. The improper rotations $i\times\delta$ where i is the inversion cannot be so represented but we may simply treat δ in the way outlined above and consider the products $i\times\delta$ using the facts that i commutes with all rotations and that $i^2=\epsilon$ even when spin is included.[11] Each of the two forms of the rotation u, which we can conveniently call u and $\bar{u}$, correspond to an ordinary rotation in Cartesian space and therefore have the same effect when operating on a vector; i.e.,

$$u\mathbf{t}=\bar{u}\mathbf{t}.$$

By using these facts the classes and the characters of the irreducible representations can be readily obtained from the well-known product, orthogonality, and normalization conditions.[12] Opechowski[7] obtained a number of simple rules which help considerably in constructing a double group from a known single point group. The most important are:

(1). If δ_n form a class of rotations through $2\pi/n$ in the single group δ_n, $\bar{\delta}_n$ form two separate classes in the double group.

(2). There is one exception to (1). If the rotations are through π $(n=2)$, then δ_2, $\bar{\delta}_2$ form one class in the double group if, and only if, there is also in the group another rotation through π about an axis perpendicular to the axis of δ_2.

(3). For the extra irreducible representations in the double group

$$\chi^d(\delta_n)=-\chi^d(\bar{\delta}_n),$$

and in the exceptional case (2), $\chi(\delta_2)=0$.

Similar rules can be constructed when the group elements are of the more general form $(\alpha|a)$.

(1). The condition above is a negative one: δ_n, $\bar{\delta}_n$ form separate classes because there is no rotation ξ in the group such that $\delta_n\xi=\xi\bar{\delta}_n$. With the addition of translations therefore rule (1) above still holds.

(2). In the exceptional case the translations impose a further condition. If there is another rotation $(\delta_2'|\tau')$ about a perpendicular axis $(\delta_2|\tau)$, $(\bar{\delta}_2|\tau)$ are only in the same class if

$$(\delta_2|\tau)(\delta_2'|\tau')=(\delta_2'|\tau')(\bar{\delta}_2|\tau),$$

i.e., if

$$(\epsilon-\delta_2')\tau=(\epsilon-\delta_2)\tau'.$$

In fact it is $(\bar{\delta}_2|t)$ which is in the same class as $(\delta_2|\tau)$ where $t=(\epsilon-\delta_2)\tau'-\delta_2'\tau$. Each class of δ_2 elements must therefore be tested carefully in this way when the double group is formed.

(3). As before when two classes are formed from one, whether in (1) or (2) the extra irreducible representations have characters which are of opposite sign. If there is only one class, the character is zero.

TIME REVERSAL

Wigner[8] has demonstrated that extra degeneracies often occur because of time-reversal symmetry. The effects of time reversal can be seen for three different cases, depending on the nature of the complex matrices D which form an irreducible representation of the group. They are:

(a) D is real.

(b) D, D^* belong to inequivalent irreducible representations.

(c) D, D^* belong to equivalent representations but are distinct.

For electrons with spin Wigner shows that for the

[11] See for example B. L. van der Waerden, *Die Gruppentheoretische Methode in der Quantenmechanik* (Verlag Julius Springer, Berlin, 1932).

[12] These are outlined in references 2 and 7. See also A. Speiser, *Theorie der Gruppen von endlicher Ordnung* (Verlag Julius Springer, Berlin, 1927).

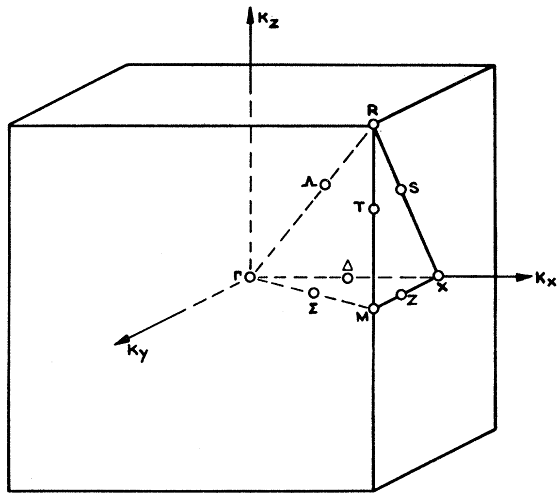

FIG. 1. First Brillouin zone for a s.c. lattice.

various cases,

(a) There is an extra degeneracy and the representation D always occurs doubled.
(b) There is extra degeneracy and the two representations D and D^* always occur together.
(c) There is no extra degeneracy.

This is different from the case when there is no spin—then the roles (a) and (c) are reversed. Herring[t] has considered the effects of this in space groups, by modification of a general theorem of Frobenius and Schur.[13] They show that in a group of N elements T for the three cases listed,

(a) $$\sum_T \chi(T^2)=N,$$
(b) $$=0,$$
(c) $$=-N.$$

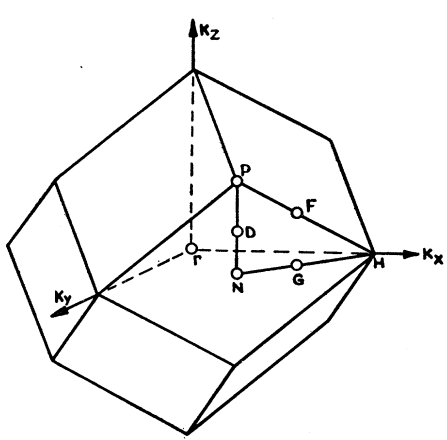

FIG. 2. First Brillouin zone for a b.c.c. lattice.

[13] G. Frobenius and I. Schur, S. B. Pruss. Akad. Wiss. 186 (1906).

For space groups this test reduces to

$$\sum_{Q_0} \chi(Q_0^2)=n,\ 0,\ \text{or}\ -n,$$

where Q_0 are those elements of G which turn $\mathbf{k}$ into $-\mathbf{k}$.
For $\mathbf{k}s$ where the inversion operation I is not in G^k the Q_0 are $I\times G^k$. If I is in G^k the Q_0 are just the elements of G^k. Q_0^2 is an element of G^k so the above χ can be taken in an irreducible representation of the group of $\mathbf{k}$ which has n elements.

At a general point in the Brillouin zone G^k/T^k contains the translation group and the identity which now corresponds to two elements ϵ and $\bar{\epsilon}$. The only Q_0 which take $\mathbf{k}$ into $-\mathbf{k}$ are the inversions $(i|\tau)$ and $(\bar{i}|\tau)$ and therefore if the group G contains the inversion,

$$\sum_{Q_0} \chi(Q_0^2)=2\chi(\epsilon)=2,$$

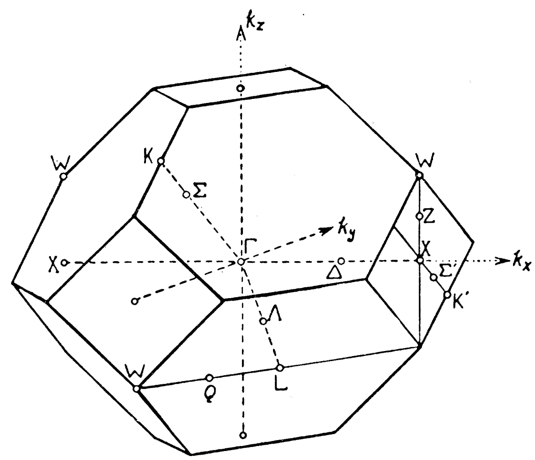

FIG. 3 First Brillouin zone for f.c.c. and diamond lattices.

which means case (a) holds and there is always a double degeneracy at the general point because of time reversal. There must always be at least a double degeneracy therefore at all points of the zone if the crystal has inversion symmetry. Any singly degenerate representations occurring at points of higher symmetry must therefore belong to cases (a) or (b). Such representations have been tested and the extra degeneracies are listed in the Tables.

When case (b) applies it is often useful to discover which are the representations of the group of $\mathbf{k}$ which correspond to the conjugate representations D, D^* of the whole group G. Let $\psi_{\mathbf{k}}{}^i$, $\psi_{\mathbf{k}'}{}^i$ form a basis for a representation of G. Then the set $\mathbf{k}'$ will include all wave vectors in the star of $\mathbf{k}$, and if as in the crystals we are discussing the group contains the inversion I, it will include $-\mathbf{k}$. The appropriate $\psi_{-\mathbf{k}}{}^i$ can be obtained from $\psi_{\mathbf{k}}{}^i$ by operating with I. The basis representing the time-reversed wave functions can be obtained by operating with Wigner's K, which consists of a unitary

TABLE I. Character table of the extra representations in the "double" group of Γ.

96		$\Gamma_6^\pm$	$\Gamma_7^\pm$	$\Gamma_8^\pm$		
1	E	2	2	4	Γ_i	$\Gamma_i\times D_{\frac{1}{2}}$
1	$\bar{E}$	−2	−2	−4	Γ_1	Γ_6^+
6	$C_4^2, \bar{C}_4^2$	0	0	0	Γ_2	Γ_7^+
6	C_4	$\sqrt{2}$	$-\sqrt{2}$	0	Γ_{12}	Γ_8^+
6	$\bar{C}_4$	$-\sqrt{2}$	$\sqrt{2}$	0	Γ_{15}'	$\Gamma_6^+ + \Gamma_8^+$
12	$C_2, \bar{C}_2$	0	0	0	Γ_{25}'	$\Gamma_7^+ + \Gamma_8^+$
8	C_3	1	1	−1	Γ_1'	Γ_6^-
8	$\bar{C}_3$	−1	−1	1	Γ_2'	Γ_7^-
48	$I\times Z$	$\pm\chi(Z)$	$\pm\chi(Z)$	$\pm\chi(Z)$	etc.	etc.

TABLE II. Character table of the extra representations in the "double" group of Δ.

16		Δ_6	Δ_7		
1	E	2	2		
1	$\bar{E}$	−2	−2	Δ_i	$\Delta_i\times D_{\frac{1}{2}}$
2	$C_4^2, \bar{C}_4^2$	0	0	Δ_1	Δ_6
2	C_4	$\sqrt{2}$	$-\sqrt{2}$	Δ_2	Δ_7
2	$\bar{C}_4$	$-\sqrt{2}$	$\sqrt{2}$	Δ_2'	Δ_7
4	$I\times C_4^2, I\times\bar{C}_4^2$	0	0	Δ_1'	Δ_6
4	$I\times C_2, I\times\bar{C}_2$	0	0	Δ_5	$\Delta_6+\Delta_7$

TABLE III. Character table of the extra representations in the "double" group of P.

48		P_6	P_7	P_8		
1	E	2	2	4	P_i	$P_i\times D^{\frac{1}{2}}$
1	$\bar{E}$	−2	−2	−4	P_1	P_6
6	$C_4^2, \bar{C}_4^2$	0	0	0	P_2	P_7
8	C_3	1	1	−1	P_3	P_8
8	$\bar{C}_3$	−1	−1	1	P_4	P_7+P_8
6	$I\times C_4$	$\sqrt{2}$	$-\sqrt{2}$	0	P_5	P_6+P_8
6	$I\times\bar{C}_4$	$-\sqrt{2}$	$\sqrt{2}$	0		
12	$I\times C_2, I\times\bar{C}_2$	0	0	0		

TABLE IV. Character table of the extra representation in the "double" group of M.

32		$M_6^\pm$	$M_7^\pm$		
1	E	2	2	M_i	$M_i\times D_{\frac{1}{2}}$
1	$\bar{E}$	−2	−2	M_1	M_6^+
4	$C_4^2, \bar{C}_4^2$	0	0	M_2	M_7^+
2	$C_4^2, \bar{C}_4^2, \perp$	0	0	M_3	M_7^+
2	$C_4, \perp$	$\sqrt{2}$	$-\sqrt{2}$	M_4	M_6^+
2	$\bar{C}_4, \perp$	$-\sqrt{2}$	$\sqrt{2}$	M_5	$M_6^+ + M_7^+$
4	$C_2, \bar{C}_2$	0	0	M_1'	M_6^-
16	$I\times Z$	$\pm\chi(Z)$	$\pm\chi(Z)$	etc.	etc.

operation U, and the operation of taking complex conjugates, i.e., it becomes $U\psi_{\mathbf{k}}^{i*}$, $U\psi_{\mathbf{k}'}^{i*}$, etc. Since we are considering character properties we may omit the U. The time-reversed functions which form a basis for the irreducible representation of the group of $\mathbf{k}$ are therefore ψ_{-k}^* or $(I\psi_k)^*$.

Now if R is any element of the group of k,

$$R\psi_{\mathbf{k}}^i = r_{ij}\psi_{\mathbf{k}}^j.$$

Operating with I and defining a translation $\mathbf{t}$ by the expression $IR=(\epsilon|t)RI$, we find

$$R\psi_{-\mathbf{k}}^i=\exp(-i\mathbf{k}\cdot\mathbf{t})r_{ij}\psi_{-\mathbf{k}}^j$$

since R is real

$$R\psi_{-\mathbf{k}}^{i*}=\exp(i\mathbf{k}\cdot\mathbf{t})r_{ij}\psi_{-\mathbf{k}}^{j*}.$$

So the character of the representation corresponding to D^* is given in terms of that corresponding to D by

$$\chi(D^*)=\exp(i\mathbf{k}\cdot\mathbf{t})\chi^*(D).$$

TABLE V. Character table of the extra representations in the "double" group of L.

24		$L_4^\pm$	$L_5^\pm$	L_6		
1	E	1	1	2	L_i	$L_i\times D_{\frac{1}{2}}$
1	$\bar{E}$	−1	−1	−2	L_1	L_6^+
2	C_3	−1	−1	1	L_2	L_6^+
2	$\bar{C}_3$	1	1	−1	L_3	$L_4^+ + L_5^+ + L_6^+$
3	C_2	i	$-i$	0	L_1'	L_6^-
3	$\bar{C}_2$	$-i$	i	0	etc.	etc.
12	$I\times Z$	$\pm\chi(Z)$	$\pm\chi(Z)$	$\pm\chi(Z)$		

L_4^+, L_5^+ and L_4^-, L_5^- are degenerate by time reversal.

TABLE VI. Character table of the extra representations in the "double" group of W.

16		W_6	W_7		
1	E	2	2	W_i	$W_i\times D_{\frac{1}{2}}$
1	$\bar{E}$	−2	−2	W_1	W_6
2	$C_4^2, \bar{C}_4^2$	0	0	W_2	W_6
4	$C_2, \bar{C}_2$	0	0	W_1'	W_7
2	$I\times C_4$	$\sqrt{2}$	$-\sqrt{2}$	W_2'	W_7
2	$I\times\bar{C}_4$	$-\sqrt{2}$	$\sqrt{2}$	W_3	W_6+W_7
4	$I\times C_4^2$	0	0		

THE SPLITTING OF DEGENERACIES BY SPIN-ORBIT COUPLING

At a general point of the zone the representation is singly degenerate in the absence of spin, but because of time reversal, becomes doubly degenerate when we introduce the two possible spin components. The only effect then will be an energy change in the band, but this will in general be small because the spin-orbit coupling energy is small compared to the band separations. At points of high symmetry in the zone the addition of spin may cause some splitting. To find out when this occurs we consider a state which transforms like a representation Γ_i of the group of $\mathbf{k}$. The spin

TABLE VII. Character table of the extra representations in the "double" group of X.

64		X_5	
1	$(\epsilon\|0)$	4	For all the single group representations
1	$(\bar{\epsilon}\|0)$	−4	X_i $(i=1, 2, 3, 4)$, $X_i\times D_{\frac{1}{2}}=X_5$.
1	$(\epsilon\|t_{xy})$	−4	
1	$(\bar{\epsilon}\|t_{xy})$	4	
60	$(\alpha\|a)$	0	
	(for all other classes of the group)		

TABLE VIII. Character table of the representations of W.[a]

64		W_1	W_2	W_3	W_4	W_5	W_6	W_7
1	$(\epsilon\|0)$	2	2	1	1	1	1	2
1	$(\bar{\epsilon}\|0)$	2	2	-1	-1	-1	-1	-2
2	$(\delta_{2z}\|0)$, $(\bar{\delta}_{2z}\|t_{xy})$	0	0	$-i$	$-i$	$-i$	$-i$	$+2i$
4	$\left\{\begin{matrix}(\delta_{2xy}\|\tau), (\bar{\delta}_{2xy}\|\tau+t_{xy}) \\ (\delta_{2\bar{x}y}\|\tau+t_{yz}), (\bar{\delta}_{2\bar{x}y}\|\tau+t_{xz})\end{matrix}\right\}$	0	0	1	1	-1	-1	0
2	$(\sigma_{4z}\|0)$, $(\sigma_{4z}^{-1}\|t_{yz})$	$(1-i)$	$-(1-i)$	$\frac{1}{\sqrt{2}}(1-i)$	$-\frac{1}{\sqrt{2}}(1-i)$	$\frac{1}{\sqrt{2}}(1-i)$	$-\frac{1}{\sqrt{2}}(1-i)$	0
2	$(\bar{\sigma}_{4z}\|0)$, $(\bar{\sigma}_{4z}^{-1}\|t_{yz})$	$(1-i)$	$-(1-i)$	$-\frac{1}{\sqrt{2}}(1-i)$	$\frac{1}{\sqrt{2}}(1-i)$	$-\frac{1}{\sqrt{2}}(1-i)$	$\frac{1}{\sqrt{2}}(1-i)$	0
4	$\left\{\begin{matrix}(\rho_x\|\tau), (\bar{\rho}_x\|\tau+t_{xy}) \\ (\rho_y\|\tau+t_{xz}), (\bar{\rho}_y\|\tau+t_{yz})\end{matrix}\right\}$	0	0	$\frac{1}{\sqrt{2}}(1+i)$	$-\frac{1}{\sqrt{2}}(1+i)$	$-\frac{1}{\sqrt{2}}(1+i)$	$\frac{1}{\sqrt{2}}(1+i)$	0
16	$(\alpha\|a)\times(\epsilon\|t_{yz})$				$-i\chi[(\alpha\|a)]$			
16	$(\alpha\|a)\times(\epsilon\|t_{xy})$				$-\chi[(\alpha\|a)]$			
16	$(\alpha\|a)\times(\epsilon\|t_{xz})$				$i\chi[(\alpha\|a)]$			

$W_1\times D_{\frac{1}{2}}=W_3+W_5+W_7$; $W_2\times D_{\frac{1}{2}}=W_4+W_6+W_7$.

W_3, W_5 and W_4, W_6 are degenerate by time reversal.

[a] Dr. Herring has pointed out that there is an error in his single group W. In order to define its representations properly, we give the characters for the single group as well.

functions transform like $D_{\frac{1}{2}}$ of the rotation group and since the spin and coordinate spaces are quite distinct we form the direct product,

$$\Gamma_i\times D_{\frac{1}{2}}=\sum a_{ij}\Gamma_j.$$

Γ_i is a representation which occurred in the single group and so it occurs in the double group also with $\chi(E)=\chi(\bar{E})$. On the other hand in $D_{\frac{1}{2}}$, $\chi(E)=-\chi(\bar{E})=2$. Therefore only those representations with $\chi(E)=-\chi(\bar{E})$ occur in the sum on the right of expression, i.e., only the new representations introduced by forming the double group. The constants a_{ij} can be readily obtained by finding the product of the characters. The character of a rotation through an angle $2\pi/n$ in $D_{\frac{1}{2}}$ is $2\cos(\pi/n)$.

It is also of interest to find out how the representation changes as we move from one point in the zone to another with different symmetry properties. To do this we construct compatability relations as defined by Bouckaert, Smoluchowski, and Wigner.[1] Various interesting sequences of these are given in the Tables. These are much fewer in number than in the single group, because most of the symmetry lines do not now have more than one available irreducible representation, and the effect of moving away from a symmetry point can be seen simply by examining the dimensions of the representation.

TABLES OF CHARACTERS

Only the extra representations which arise in the double group are given in these Tables. To avoid confusion the same notation is used as in the papers where the single group character Tables are given. When the group is a direct product, the Tables have been shortened by writing the products $(\alpha|a)\times(\gamma|c)$ where $(\alpha|a)$ are all the elements already listed. To

TABLE IX. Character table of the extra representations in the "double" group of $\Delta(X)$.

32		$\Delta_6(X)$	$\Delta_7(X)$		
1	$(\epsilon\|0)$	2	2	Δ_i	$\Delta_i\times D_{\frac{1}{2}}$
1	$(\bar{\epsilon}\|0)$	-2	-2	Δ_1	Δ_6
2	$(\delta_{2x},\bar{\delta}_{2x}\|0)$	0	0	Δ_1'	Δ_6
2	$(\delta_{4x},\delta_{4x}^{-1}\|\tau)$	$-\sqrt{2}i$	$\sqrt{2}i$	Δ_2	Δ_7
2	$(\bar{\delta}_{4x},\bar{\delta}_{4x}^{-1}\|\tau)$	$\sqrt{2}i$	$-\sqrt{2}i$	Δ_2'	Δ_7
4	$(\rho_z,\bar{\rho}_z,\rho_y,\bar{\rho}_y\|\tau)$	0	0	Δ_5	$\Delta_6+\Delta_7$
4	$(\rho_{yz},\bar{\rho}_{yz},\rho_{\bar{y}z},\bar{\rho}_{\bar{y}z}\|0)$	0	0		
16	$(\alpha\|a)\times(\epsilon\|t_{xy})$	$-\chi[(\alpha\|a)]$			

TABLE X. Character table of the extra representations in the "double" group of $Z(X)$.

16		Z_2	Z_3	Z_4	Z_5
1	$(\epsilon\|0)$	1	1	1	1
1	$(\epsilon\|t_{xy})$	-1	-1	-1	-1
2	$(\delta_{2z}\|0)$, $(\bar{\delta}_{2z}\|t_{xy})$	i	i	$-i$	$-i$
2	$(\rho_x\|\tau)$, $(\bar{\rho}_x\|\tau+t_{xy})$	i	$-i$	i	$-i$
2	$(\rho_y\|\tau)$, $(\bar{\rho}_y\|\tau+t_{xy})$	-1	1	1	-1
8	$(\alpha\|a)\times(\bar{\epsilon}\|0)$		$-\chi[(\alpha\|a)]$		

$Z_1\times D_{\frac{1}{2}}=Z_2+Z_3+Z_4+Z_5$

Z_2, Z_3 and Z_4, Z_5 are degenerate by time reversal.

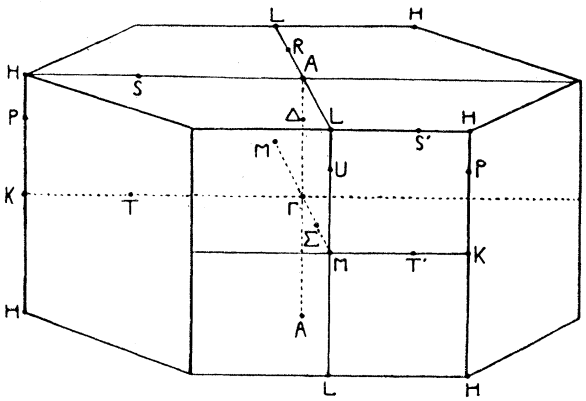

FIG. 4. First Brillouin zone for h.c.p. lattice.

every class listed there will be a further class in this product. The character of the product is given in terms of the character of $(\alpha|a)$ already listed.

Simple, Face-Centered, and Body-Centered Cubic Lattices

For the s.c., f.c.c., and b.c.c. lattices[1] we need only consider point groups and we give Tables I–VI for the positions Γ, Δ, P, M, L, and W and others which are isomorphous with them. The double groups of Λ, F, Σ, S, Z, G, K, U, D, Q, are trivial since the only extra representation is one where $\chi(E)=2$, $\chi(\bar{E})=-2$, $\chi(C)=0$, where C is any rotation, and the wave functions of all bands transform in the same way. This representation is the same as the one for the general **k** which we have seen is double by time reversal. For N there are two extra representations one of which is even and the other odd with respect to the inversion, so the results are again trivial. The positions of the symmetry points can be seen by reference to the Figs. 1–3 which are the first Brillouin zones of the s.c., b.c.c., and f.c.c. lattices, respectively.

Δ is the only symmetry line where the representations are nontrivial, and we need therefore only consider

TABLE XI. Character table of the extra representations in the "double" group of A and Γ.

96		A_4	A_5	A_6	$\Gamma_7^{\pm}$	$\Gamma_8^{\pm}$	$\Gamma_9^{\pm}$
1	$(\epsilon\|0)$	2	2	4	2	2	2
1	$(\bar{\epsilon}\|0)$	−2	−2	−4	−2	−2	−2
1	$(\epsilon\|t_{xy})$	−2	−2	−4			
1	$(\bar{\epsilon}\|t_{xy})$	2	2	4			
4	$(\delta_6,\delta_6^{-1}\|\tau,\tau+t_1)$	0	0	0	$\sqrt{3}$	$-\sqrt{3}$	0
4	$(\bar{\delta}_6,\bar{\delta}_6^{-1}\|\tau,\tau+t_1)$	0	0	0	$-\sqrt{3}$	$\sqrt{3}$	0
2	$(\delta_3,\delta_3^{-1}\|0)$	−2	−2	2	1	1	−2
2	$(\bar{\delta}_3,\bar{\delta}_3^{-1}\|0)$	2	2	−2	−1	−1	2
2	$(\delta_3,\delta_3^{-1}\|t_1)$	2	2	−2			
2	$(\bar{\delta}_3,\bar{\delta}_3^{-1}\|t_1)$	−2	−2	2			
4	$(\delta_2,\bar{\delta}_2\|\tau,\tau+t_1)$	0	0	0	0	0	0
6	$(\delta_{2i}'\|\tau)$, $(\bar{\delta}_{2i}'\|\tau+t_1)$	$2i$	$-2i$	0	0	0	0
6	$(\bar{\delta}_{2i}'\|\tau)$, $(\delta_{2i}'\|\tau+t_1)$	$-2i$	$2i$	0			
12	$(\delta_{2i}'',\bar{\delta}_{2i}''\|\tau,\tau+t_1)$	0	0	0	0	0	0
2	$(i\|\tau,\tau+t_1)$	0	0	0	±2	±2	±2
2	$(\bar{i}\|\tau,\tau+t_1)$	0	0	0	∓2	∓2	∓2
4	$(\sigma_3,\sigma_3^{-1}\|0,t_1)$	0	0	0	$\pm\sqrt{3}$	$\mp\sqrt{3}$	0
4	$(\bar{\sigma}_3,\bar{\sigma}_3^{-1}\|0,t_1)$	0	0	0	$\mp\sqrt{3}$	$\pm\sqrt{3}$	0
4	$(\sigma_6,\sigma_6^{-1}\|\tau,\tau+t_1)$	0	0	0	±1	±1	∓2
4	$(\bar{\sigma}_6,\bar{\sigma}_6^{-1}\|\tau,\tau+t_1)$	0	0	0	∓1	∓1	±2
4	$(\rho,\bar{\rho}\|0,t_1)$	0	0	0	0	0	0
6	$(\rho_i',\bar{\rho}_i'\|0)$	0	0	0	0	0	0
6	$(\rho_i',\bar{\rho}_i'\|t_1)$	0	0	0			
12	$(\rho_i'',\bar{\rho}_i''\|\tau,\tau+t_1)$	0	0	0	0	0	0

A_4, A_5 are degenerate by time reversal.

Γ_i	$\Gamma_1^{\pm}$	$\Gamma_2^{\pm}$	$\Gamma_3^{\pm}$	$\Gamma_4^{\pm}$	$\Gamma_5^{\pm}$	$\Gamma_6^{\pm}$	A_1	A_2	A_3
$\Gamma_i\times D_{\frac{1}{2}}$	$\Gamma_7^{\pm}$	$\Gamma_7^{\pm}$	$\Gamma_8^{\pm}$	$\Gamma_8^{\pm}$	$\Gamma_7^{\pm}+\Gamma_9^{\pm}$	$\Gamma^{\pm}+\Gamma_9^{\pm}$	A_6	A_6	$A_4+A_5+A_6$

TABLE XII. Character table of the extra representations in the "double" group of L and M.

64		L_3	L_4	$M_5^{\pm}$
1	$(\epsilon\|0)$	2	2	2
1	$(\bar{\epsilon}\|0)$	−2	−2	−2
1	$(\epsilon\|t_1)$	−2	−2	
1	$(\bar{\epsilon}\|t_1)$	2	2	
2	$(\delta_{2z}'\|\tau_2)$, $(\bar{\delta}_{2z}'\|\tau_2+t_1)$	$2i$	$-2i$	0
2	$(\bar{\delta}_{2z}'\|\tau_2)$, $(\delta_{2z}'\|\tau_2+t_1)$	$-2i$	$2i$	
4	$(\delta_{2z}'',\bar{\delta}_{2z}''\|0,t_1)$	0	0	0
4	$(\delta_2, \bar{\delta}_2\|\tau_2, \tau_2+t_1)$	0	0	0
2	$(i\|\tau_2, \tau_2+t_1)$	0	0	±2
2	$(\bar{i}\|\tau_2, \tau_2+t_1)$	0	0	∓2
2	$(\rho_2',\bar{\rho}_2'\|0)$	0	0	0
2	$(\rho_2',\bar{\rho}_2'\|t_1)$	0	0	
4	$(\rho_2'', \bar{\rho}_2''\|\tau_2, \tau_2+t_1)$	0	0	0
4	$(\rho,\bar{\rho}\|0,t_1)$	0	0	0
32	$(\alpha\|a)\times(\epsilon\|t_3)$	$-\chi[(\alpha\|a)]$		$-\chi[(\alpha\|a)]$

$L_1\times D_{\frac{1}{2}}=L_2\times D_{\frac{1}{2}}=L_3+L_4$

For all $M_i^{\pm}$ ($i=1$, 2, 3, 4) $M_i^{\pm}\times D_{\frac{1}{2}}=M_5^{\pm}$

L_3, L_4 are degenerate by time reversal.

TABLE XIII. Character table of the extra representations in the "double" group of H and K.

144		H_4	H_5	H_6	H_7	H_8	H_9	K_7	K_8	K_9
1	$(\epsilon\|0)$	1	1	1	1	2	2	2	2	2
1	$(\epsilon\|t_1)$	-1	-1	-1	-1	-2	-2			
2	$(\delta_3\|t_2)$, $(\delta_3^{-1}\|-t_2)$	-1	-1	-1	-1	1	1	1	1	-2
2	$(\delta_3\|t_1+t_2)$, $(\delta_3^{-1}\|-t_1-t_2)$	1	1	1	1	-1	-1			
6	$(\delta_{2i}'\|\tau_i)$, $(\bar{\delta}_{2i}'\|\tau_1+t_1)$	i	i	$-i$	$-i$	0	0	0	0	0
2	$(\sigma_3\|-t_2)$, $(\sigma_3^{-1}\|t_1+t_2)$	i	$-i$	i	$-i$	i	$-i$	$\sqrt{3}$	$-\sqrt{3}$	0
2	$(\sigma_3\|-t_1-t_2)$, $(\sigma_3^{-1}\|t_2)$	$-i$	i	$-i$	i	$-i$	i			
2	$(\rho\|0)$, $(\bar{\rho}\|t_1)$	$-i$	i	$-i$	i	$2i$	$-2i$	0	0	0
6	$(\rho_i''\|\tau_i)$, $(\bar{\rho}_i''\|\tau_i+t_1)$	1	-1	-1	1	0	0	0	0	0
24	$(\alpha\|a)\times(\bar{\epsilon}\|0)$			$-\chi[(\alpha\|a)]$					$-\chi[(\alpha\|a)]$	
48	$(\gamma\|c)\times(\epsilon\|t_2)$			$\omega\chi[(\gamma\|c)]$					$\omega\chi[(\gamma\|c)]$	
48	$(\gamma\|c)\times(\epsilon\|-t_2)$			$\omega^2\chi[(\gamma\|c)]$					$\omega^2\chi[(\gamma\|c)]$	

H_i	H_1	H_2	H_3	K_1	K_2	K_3	K_4	K_5	K_6
$H_i\times D_{\frac{1}{2}}$	H_8+H_9	$H_4+H_6+H_8$	$H_5+H_7+H_9$	K_7	K_8	K_7	K_8	K_8+K_9	K_7+K_9

H_4, H_6 and H_5, H_7 are degenerate by time reversal.

TABLE XIV. Character table of the extra representations in the "double" group of Δ.

48		$\Delta_7(A)$	$\Delta_8(A)$	$\Delta_9(A)$	$\Delta_7(\Gamma)$	$\Delta_8(\Gamma)$	$\Delta_9(\Gamma)$
1	$(\epsilon\|0)$	2	2	2	2	2	2
1	$(\bar{\epsilon}\|0)$	-2	-2	-2	-2	-2	-2
2	$(\delta_6,\delta_6^{-1}\|\tau)$	$-\sqrt{3}i$	$+\sqrt{3}i$	0	$\sqrt{3}$	$-\sqrt{3}$	0
2	$(\bar{\delta}_6,\bar{\delta}_6^{-1}\|\tau)$	$+\sqrt{3}i$	$-\sqrt{3}i$	0	$-\sqrt{3}$	$\sqrt{3}$	0
2	$(\delta_3,\delta_3^{-1}\|0)$	1	1	-2	1	1	-2
2	$(\bar{\delta}_3,\bar{\delta}_3^{-1}\|0)$	-1	-1	2	-1	-1	2
2	$(\delta_2,\bar{\delta}_2\|0)$	0	0	0	0	0	0
6	$(\rho_i',\bar{\rho}_i'\|0)$	0	0	0	0	0	0
6	$(\rho_i'',\bar{\rho}_i''\|\tau)$	0	0	0	0	0	0
24	$(\alpha\|a)\times(\epsilon\|t_1)$		$-\chi[(\alpha\|a)]$				

Δ_i	$\Delta_i\times D_{\frac{1}{2}}$
Δ_1	Δ_7
Δ_2	Δ_8
Δ_3	Δ_7
Δ_4	Δ_8
Δ_5	$\Delta_7+\Delta_9$
Δ_6	$\Delta_8+\Delta_9$

its compatibility relations: $\Gamma_{6^\pm}\rightarrow\Delta_6$, $\Gamma_{7^\pm}\rightarrow\Delta_7$, and $\Gamma_{8^\pm}\rightarrow\Delta_6+\Delta_7$; $M_6\rightarrow\Delta_6$. $M_7\rightarrow\Delta_7$.

Diamond Lattice

We shall use throughout the notation adopted by Herring.[2] The lattice has the same translational symmetry as the face-centered cubic, but its unit cell is more complicated since it contains two atoms and therefore the cell group contains screw elements. Even so some of the groups are isomorphous with those of the f.c.c. lattice, and we need not consider them again. The exact correspondence of the elements is discussed by Herring. The groups for the points X and W, and the lines Δ and Z are however different. We evaluate the double groups of these in the limit as they approach X. The first Brillouin zone is equivalent to that for f.c.c. (Fig. 2).

The lines of symmetry Δ and Z in this lattice have nontrivial compatibility relations: $\Gamma_6^\pm\rightarrow\Delta_6(\Gamma)$, $\Gamma_7^\pm\rightarrow\Delta_7(\Gamma)$, $\Gamma_8^\pm\rightarrow\Delta_6(\Gamma)+\Delta_7(\Gamma)$, and $X_5\rightarrow\Delta_6(X)+\Delta_7(X)$. $X_5\rightarrow Z_2+Z_3+Z_4+Z_5$, $W_3+W_5\rightarrow Z_4+Z_5$, $W_4+W_6\rightarrow Z_4+Z_5$, $W_7\rightarrow Z_2+Z_3$.

TABLE XV. Character table of the extra representations in the "double" group of P.

72		$P_4(H)$	$P_5(H)$	$P_6(H)$	$P_4(K)$	$P_5(K)$	$P_6(K)$
1	$(\epsilon\|0)$	1	1	2	1	1	2
2	$(\delta_3\|t_2)$, $(\delta_3^{-1}\|-t_2)$	-1	-1	1	-1	-1	1
3	$(\rho_i''\|\tau_i)$	1	-1	0	$-i$	i	0
6	$(\alpha\|a)\times(\bar{\epsilon}\|0)$		$-\chi[(\alpha\|a)]$			$-\chi[(\alpha\|a)]$	
12	$(\gamma\|c)\times(\epsilon\|t_2)$		$\omega\chi[(\gamma\|c)]$			$\omega\chi[(\gamma\|c)]$	
12	$(\gamma\|c)\times(\epsilon\|-t_2)$		$\omega^2\chi[(\gamma\|c)]$			$\omega^2\chi[(\gamma\|c)]$	
36	$(\beta\|b)\times(\epsilon\|t_1)$		$-\chi[(\beta\|b)]$				

P_4, P_5 are degenerate by time reversal,
$P_1\times D_{\frac{1}{2}}=P_2\times D_{\frac{1}{2}}=P_6$ $P_3\times D_{\frac{1}{2}}=P_4+P_5+P_6$

TABLE XVI. Character table of the extra representations in the "double" group of S.

16		S_2	S_3	S_4	S_5
1	$(\epsilon\|0)$	1	1	1	1
1	$(\epsilon\|t_1)$	-1	-1	-1	-1
2	$(\delta_{2z}'\|\tau_2)$, $(-\bar{\delta}_{2z}'\|\tau_2+t_1)$	i	i	$-i$	$-i$
2	$(\rho\|0)$, $(\bar{\rho}\|t_1)$	$-i$	i	i	$-i$
2	$(\rho_2''\|\tau_2)$, $(\bar{\rho}_2''\|\tau_2+t_1)$	1	-1	1	-1
8	$(\alpha\|a)\times(\bar{\epsilon}\|0)$		$-\chi[(\alpha\|a)]$		

$S_1\times D_{\frac{1}{2}}=S_2+S_3+S_4+S_5$
S_3, S_4 and S_2, S_5 are degenerate by time reversal.

Hexagonal Close-Packed Lattice

We shall again follow exactly the notation of Herring.[2] The first Brillouin zone and the various kinds of symmetry point are shown in Fig. 4.

The double groups of U, Σ, R, and T are trivial; there being only one extra representation which has zero character for everything except the identity ($\chi(\epsilon)=-\chi(\bar{\epsilon})=2$) and translations. This representation of R, however, always occurs twice because of time reversal so the states are all fourfold degenerate on R. The only other symmetry position S has character Table XVI.

Depending on the limiting position of the point S we should also consider primary translations in the group of S. This would give the same results as in Herring's single tables and they are omitted here.

The compatibility relations for the lines Δ, P and S are nontrivial: $\Gamma_i^{\pm}\rightarrow\Delta_i(\Gamma)$ ($i=7$, 8, 9). $A_4\rightarrow\Delta_9(A)$, $A_5\rightarrow\Delta_9(A)$, $A_6\rightarrow\Delta_7(A)+\Delta_8(A)$. H_4+H_6, $H_5+H_7\rightarrow P_4(H)+P_5(H)$; H_8, $H_9\rightarrow P_6(H)$. K_7, $K_8\rightarrow P_6(K)$; $K_9\rightarrow P_4(K)+P_5(K)$. A_4+A_5, $A_6\rightarrow S_2(A)+S_3(A)+S_4(A)+S_5(A)$. $H_4\rightarrow S_2(H)$, $H_5\rightarrow S_3(H)$, $H_6\rightarrow S_5(H)$. $H_7\rightarrow S_4(H)$, $H_8\rightarrow S_3(H)+S_4(H)$, $H_9\rightarrow S_2(H)+S_5(H)$.

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Magnetization of Tin at the Superconducting Transition

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Measurements have been made of the steady-state magnetization of a tin cylinder in the presence of an external magnetic field and with an externally supplied current at the transition to superconduction. In accord with earlier work in Germany, a longitudinal flux in excess of that caused by the external field is observed for certain combinations of external field and current. The dependence of the effect on the external parameters is given and it is shown that the metal is not in the pure superconducting state. No satisfactory theory for the effect has been found, but some numerical relationships have been computed.

INTRODUCTION

SUPERCONDUCTION in metals is an electronic state characterized by zero electrical field and by zero magnetic induction. The independent variables which may determine whether a metal is in the superconducting state, if it becomes one at all, are the temperature T, the magnetic field B, and finally because a current in the specimen may produce its own field, we must consider the current I, as a variable. At sufficiently low values of each of these variables, the metal may be in the superconducting state; just how low is a characteristic of each superconductor.[1] In this research we dealt with very pure monocrystalline tin made in the form of a cylinder and we were concerned with some unusual properties just at the transition into and out of the superconducting state. At a temperature just below the zero field transition temperature for ordinary tin, 3.735°K, and in a small externally created magnetic field of 1 to 4×10^{-4} weber/sq meter applied along the long axis of the cylinder, a steady current of from 1 to 13 amperes was allowed to flow along the cylinder and we measured the magnetic flux content of the tin specimen. The work of Steiner[2] and of Meissner, Schmeissner, and Meissner[3] has shown that under these conditions the longitudinal flux through a conductor, instead of decreasing monotonically to zero at the transition to superconduction, first shows an *increase* provided one uses certain conditions of a large current, a small external magnetic field, and a temperature such that with the currents and fields used the super to normal transition may be effected. The results which we now report are in accord with the above authors and represent a continuation of the preliminary studies by Mendelssohn, Squire, and Teasdale[4] and by Teasdale and Rorschach.[5] Dr. Mendelssohn suggested these studies and indicated the method of measurement which we have continued to use since his work with us here in this laboratory. The present apparatus has

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