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Energy Bands in the Body-Centered Lattice*

MARVIN I. CHODOROW AND MILLARD F. MANNING**
Massachusetts Institute of Technology, Cambridge, Massachusetts

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Slater's method of finding the structure of electronic energy bands in the body-centered lattices is extended so as to satisfy boundary conditions at fourteen points of the polyhedral cell surrounding an atom, instead of eight as in previous applications. Since this requires the use of all the "d" spherical harmonics, the method is now applicable to elements which have "d" electrons. Greater accuracy is also to be expected for other elements. The expansions of the determinants relating the energy E to k, the wave number vector, are given for all symmetry axes, and points, and in part for the symmetry planes. From group theory the places where various bands will stick together, i.e. degeneracies required by symmetry, are also determined.

I. INTRODUCTION

SLATER'S[1] extension of the method of Wigner and Seitz[2] has made possible an approximate determination of the detailed structure of electronic energy bands in crystals. In this method the crystal is divided into polyhedral cells of equal size, each cell surrounding one atom. In any one cell the wave function for an electron can be expanded as

$$\Psi=\sum_{m=-l}^{l}\sum_{l=0}^{\infty}A_{ml}u_lP_l^m(\cos\theta)e^{im\varphi},$$

where the u_l are radial functions (obtained by numerical integration) and $P_l^m(\cos\theta)e^{im\varphi}$ are surface harmonics. The constants A_{ml} are determined from the known periodicity conditions which the wave function and its slope must obey in a translation from one face of the cell to the perpendicularly opposite face. Since, to fulfill these conditions for the whole surface of the cell would be very difficult, in practice the boundary conditions are satisfied only at the midpoints of the faces, in which case we represent the wave function by a finite number of terms out of the above series. More exactly if we write

$$\Psi=G+iU,$$

where G is even with respect to inversion through the origin (taken at the nucleus in the center of the cell) and U is odd then the equations determining the A_{ml} are

$$U=\tan(K\cdot r_n/2)G,$$
$$G'=-\tan(K\cdot r_n/2)U'.$$

Here $r_n/2$ is the radius vector to the midpoint of one of the cell faces ($|r_n|$ is distance between midpoints of opposite faces), K is the reduced wave number vector,[3] the (′) denotes differentiation with respect to r, U, G, U', G' are evaluated at $r_n/2$. There is a pair of these equations for each pair of midpoints and therefore we will use as many terms in our polynomial for Ψ as the number of midpoints at which we wish to satisfy the boundary conditions.

These equations for A_{ml} are homogeneous and for a non-trivial solution the determinant of their coefficients must vanish. Setting this determinant equal to zero gives a relation between the energy E, which enters as a parameter in the numerical integration of the radial functions, and the wave vector K. A knowledge of E as a function of K throughout the whole Brillouin zone completely determines the structure of the band.

In previous applications to the body-centered lattice,[1, 4] in which the cell is the familiar truncated octahedron with fourteen faces, eight between nearest neighbors, and six between second nearest neighbors, the boundary conditions were satisfied at the midpoints of the faces between nearest neighbors. The eight functions

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** Now at Toledo University.

[1] J. C. Slater, Phys. Rev. **45**, 794 (1934).

[2] Wigner and Seitz, Phys. Rev. **43**, 804 (1933) and **46**, 509 (1934).

[3] Cf. A. Sommerfeld and H. Bethe, *Handbuch der Physik*, Vol. 24; J. C. Slater, Rev. Mod. Phys. **6**, 209 (1934); Mott and Jones, *Theory of the Properties of Metals and Alloys*, Oxford, 1936.

[4] J. Millman, Phys. Rev. **47**, 286 (1935). F. Seitz, Phys. Rev. **47**, 400 (1935).

used in the expansion of Ψ were one s, three p, three d, and one f. Since the group[5] of a general K vector contains only the identity operation, there is no spatial degeneracy as in a free atom and an electronic level with a given l value in the free atom, which is always $2l+1$ fold spatially degenerate, splits up into $2l+1$ bands in the crystal. However, one cannot obtain, for instance, the five bands arising from an electronic d level, if an eight term polynomial is used for Ψ, containing only three d functions. Slater[1] pointed out that the method could be extended by fitting the boundary conditions at the midpoints of the six faces between second nearest neighbors, in which case fourteen functions would be used, including all of the d functions. When the d band in the metal is occupied, it is obviously necessary to use these extra functions and even for other cases, it should improve the accuracy of the results.[6] Moreover, Shockley,[7] in an attempt to check the accuracy of the method, has shown that although the use of eight functions gave quite good results in the first zone, it was in error by about 25 percent in the second. The more elaborate method would undoubtedly give more accurate results for the higher bands, and should therefore be used even for elements having only s and p valence electrons.

II. METHOD

For a general direction of propagation, the wave function for the value of K will contain all fourteen terms, and the resulting determinant will be of the fourteenth order, which is much too unwieldy for practical computation. For special directions of propagation (in symmetry planes, or along symmetry lines of the cell), i.e., where the group of K contains more than the identity operation, the wave functions will have symmetry properties which can be used to split the determinant into smaller ones. Under the operations of the group of K, the wave functions will transform by the irreducible representations of the group, and only those spherical harmonics which belong to the same representation will appear in the expansion of any one wave function. Due to these transformation properties of the wave functions, satisying the boundary conditions on one pair of faces, automatically satisfies them on all other pairs arising from the given pair by the symmetry operations of the group. Also for some representations the transformation properties are such that either the odd or even functions, or both, must vanish on certain pairs of faces, e.g., in the case of a symmetry plane, where the group contains two elements, those functions belonging to the antisymmetric representation must obviously vanish at all points lying in the plane. All this results in reducing the number of equations necessary to fit boundary conditions on all the faces, to exactly the number of spherical harmonics (out of the fourteen) belonging to the given representation. Therefore, instead of solving a fourteenth order determinant for all the K values (corresponding to the various zones) going with a given E, we solve several much smaller determinants, each for the K value or values,[8] corresponding to the zone (or zones) belonging to that representation.[9] Since, ultimately the constant energy surfaces in the Brillouin zones

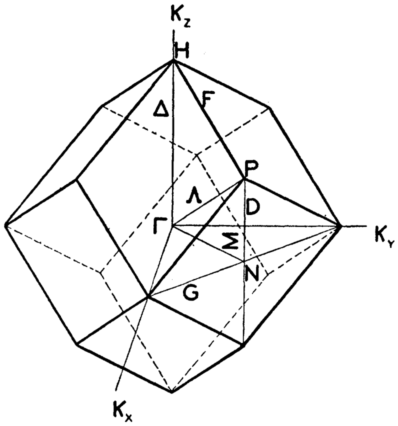

FIG. 1. Reduced Brillouin zone for the body-centered lattice.

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[5] The group of a wave vector K contains those symmetry operations of the crystal class, i.e., rotations and reflections, which either leave the vector invariant or transform it into one belonging to an equivalent irreducible representation of the translation group, i.e., a vector differing from K by one of the translations of the reciprocal lattice. Cf. F. Seitz, Ann. Math. **37**, 17 (1936); Bouckaert, Smoluchowski and Wigner, Phys. Rev. **50**, 58 (1936).

[6] Unpublished calculations on potassium show that this improvement is appreciable.

[7] Doctoral thesis, M. I. T. (1936). Shockley applied the method to a case where the wave functions and energy were known exactly (constant potential) and compared the results obtained with those of the exact treatment.

[8] For some directions several zones may belong to the same irreducible representation.

[9] For classification of Brillouin zones according to their representations see paper by B. S. W. (reference 5).

are obtained by interlopation between known directions of K, as many possible directions as give manageable determinants must be examined. In the following section we give the results obtained.

III. Results

The reduced Brillouin zone for the body-centered lattice is shown in Fig. 1. For convenience we have used the notation of Bouckaert, Smoluchowski and Wigner[5] (to be referred to as B.S.W.) in labeling the axes of symmetry. We shall also use their notation for the various irreducible representations. For any direction of K, the functions are listed according to the representation to which they belong, the dimension of the representation,[10] and the expansion of the corresponding determinant given.

As has been pointed out by B.S.W., if we pass from a point of symmetry to an axis of symmetry, the group of the latter must be a sub-group of that of the former. The irreducible representations of the group of the point considered as representations of the sub-group (group of the axis), must either be irreducible representations of the group of the axis, or (if reducible) have the latter as their irreducible parts. The irreducible representation of any band along the axis must be contained in the irreducible representation of that band at the symmetry point. Since a point of symmetry always occurs at the intersection of two or more axes of symmetry, the above compatability relations between axes and points indicate which of the various band sections along the several axes may join. However, an irreducible representation along an axis may be compatible with several different irreducible representations at a point, and therefore this joining is not completely determined by symmetry, which only limits the possibilities, the actual numerical values being necessary for a complete determination. But inasmuch as these compatibility relations may not be violated, they serve as a valuable check on any numerical calculations. For this reason we include the representations at the various symmetry points, the functions belonging to them and the determinants. We have also given these data for the symmetry planes, $K_z=0$, $K_x=K_y$, but only for the antisymmetrical representations. The determinants for the symmetrical representations are larger than can be conveniently handled.[11]

The fourteen functions used were

$$\text{even}\quad 1s\quad \frac{xy}{r^2}d\quad \frac{xz}{r^2}d\quad \frac{yz}{r^2}d\quad \frac{x^2-y^2}{r^2}d\quad \frac{3z^2-r^2}{r^2}d$$

$$\frac{5(x^4+y^4+z^4)-3r^4}{r^4}g\,;$$

$$\text{odd}\quad \frac{x}{r}p\quad \frac{y}{r}p\quad \frac{z}{r}p\quad \frac{x(5x^2-3r^2)}{r^3}f\quad \frac{y(5y^2-3r^2)}{r^3}f$$

$$\frac{z(5z^2-3r^2)}{r^3}f\quad \frac{xyz}{r^3}f\,;$$

s, p, d, f, g, refer to corresponding radial functions.

In using fourteen points we need the value of the radial functions and their slopes at two distances.

r_1 = half-distance between nearest neighbors $=(3)^{\frac{1}{2}}a/4$,

r_2 = half-distance between second nearest neighbors $=a/2$,

thus s_1, p_1, d_1, f_1, g_1, and s_1', p_1' d_1' f_1', g_1' will refer to value of the functions and slopes at the distance r_1, and s_2, f_2, etc. will refer to distance r_2. For convenience we shall use an abbreviated notation for the spherical harmonics omitting the denominator, thus x will mean x/r, $3z^2-1$ will mean $(3z^2-r^2)/r^2$ etc.

Also since certain symmetrical combinations of terms frequently appear in the expansions, we list these and the notation we use for them

$$\begin{aligned}
\sqrt{3}B_1&=3p_1'f_2'+2p_2'f_1', & S_1&=3s_1'g_2'+2s_2'g_1',\\
\sqrt{3}B_2&=3p_1'f_2+2p_2f_1', & S_2&=3s_1'g_2+2s_2g_1',\\
\sqrt{3}B_3&=3p_1f_2'+2p_2'f_1, & S_3&=3s_1g_2'+2s_2'g_1,\\
\sqrt{3}B_4&=3p_1f_2+2p_2f_1, & S_4&=3s_1g_2+2s_2g_1,\\
B_5&=p_1'f_1-p_1f_1', & S_5&=s_1'g_1-s_1g_1',\\
B_6&=p_2'f_2-p_2f_2', & S_6&=s_2'g_2-s_2g_2',
\end{aligned}$$

$$D_1=d_1'/d_1,\quad D_2=d_2'/d_2,\quad F=f_1'/f_1.$$

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[10] As in the case of atomic levels an n-dimensional irreducible representation denotes an n-fold degeneracy.

[11] Shockley (Phys. Rev. **51**, 132–3 (1937)) has given a method for expanding such determinants by using the expansions along axes contained in the plane. In our case, however, the resulting transcendental equations would be much too complicated to solve without excessive calculations.

TABLE I. *Symbol of the representation, the degeneracy (in parentheses), the functions belonging to the representation and the expanded determinant.*

Point Γ	$K=(0,0,0)$	
Γ_1	$1s$ $\{5(x^4+y^4+z^4)-3\}g$	$S_1=0$
$\Gamma_{15}(3)$	xp yp zp $x(5x^2-3)f$ $y(5y^2-3)f$ $z(5z^2-3)f$	$B_4=0$
$\Gamma_{25}'(3)$	xyd xzd yzd	$d_1'=0$
$\Gamma_{12}(2)$	$(3z^2-1)d$ $(x^2-y^2)d$	$d_2'=0$
Γ_2'	$xyzf$	$f_1=0$
Point H	$K=(0,0,2\pi/a)$	
H_1	$1s$ $\{5(x^4+y^4+z^4)-3\}g$	$S_3=0$
$H_{15}(3)$	xp yp zp $x(5x^2-3)f$ $y(5y^2-3)f$ $z(5z^2-3)f$	$B_2=0$
$H_{25}'(3)$	xyd xzd yzd	$d_1=0$
$H_{12}(2)$	$(3z^2-1)d$ $(x^2-y^2)d$	$d_2=0$
H_2'	$xyzf$	$f_1'=0$
Point P	$K=(\pi/a,\pi/a,\pi/a)$	
P_1	$1s$ $\{5(x^4+y^4+z^4)-3\}g$ $xyzf$	$FS_4+S_2=0$
$P_3(2)$	$(3z^2-1)d$ $(x^2-y^2)d$	$d_2=0$
$P_4(3)$	xp yp zp xyd xzd yzd $x(5x^2-3)f$ $y(5y^2-3)f$ $z(5z^2-3)$	$D_1B_3+B_1=0$
Point N	$K=(\pi/a,\pi/a,0)$	
N_1	$1s$ xyd $(3z^2-1)d$ $\{5(x^4+y^4+z^4)-3\}g$	$2D_1D_2S_4+2D_2S_2+D_1S_3+S_1=0$
N_2	$(xz-yz)d$	$d_1'=0$
N_3	$(xz+yz)d$	$d_1=0$
N_4	$(x^2-y^2)d$	$d_2=0$
N_1'	$(x+y)p$ $\{x(5x^2-3)+y(5y^2-3)\}f$	$B_1=0$
N_3'	zp $z(5z^2-3)f$ $xyzf$	$FB_4+B_2=0$
N_4'	$(x-y)p$ $\{x(5x^2-3)-y(5y^2-3)\}f$	$B_3=0$
Line Δ	$K=(0,0,k)$ $T_1=\tan(ka/4)$ $T_2=\tan(ka/2)$	
Δ_1	$1s$ zp $(3z^2-1)d$ $z(5z^2-3)f$ $\{5(x^4+y^4+z^4)-3\}g$	$T_2^2T_1^2B_1(2S_3+D_2S_4)-6T_2T_1D_2(S_5B_6+S_6B_5)+T_2^2B_3(2S_1+D_2S_2)+3T_1^2B_2D_2S_3+3D_2B_4S_1=0$
Δ_2	$(x^2-y^2)d$	$d_2'=0$
Δ_2'	xyd $xyzf$	$FT_1^2+D_1=0$
$\Delta_5(2)$	xp yp xzd yzd $x(5x^2-3)f$ $y(5y^2-3)f$	$B_2T_1^2+D_1B_4=0$
Line Σ	$K=(k,k,0)$ $T=\tan(ka/2)$	
Σ_1	$1s$ $(x+y)p$ xyd $(3z^2-1)d$ $\{x(5x^2-3)+y(5y^2-3)\}f$ $\{5(x^4+y^4+z^4)-3\}g$	$T^4B_1(2D_1D_2S_4+D_1S_3+2D_2S_2+S_1)+T^2\{3D_2B_2(S_1+D_1S_3)+2D_1B_3(2D_2S_2+S_1)-12B_6S_5D_1D_2-12B_5S_6D_1D_2\}+6D_1D_2S_1B_4=0$
Σ_2	$(xy-yz)d$	$d_1'=0$
Σ_3	zp $(xz+yz)d$ $z(5z^2-3)f$ $xyzf$	$T^2(B_2+FB_4)+2D_1B_4=0$
Σ_4	$(x-y)p$ $(x^2-y^2)d$ $\{x(5x^2-3)-y(5y^2-3)\}$	$T^2B_3+D_2B_4=0$

In Table I we list first the symbol of the representation, in parentheses the degeneracy, if any, then the functions belonging to that representation and the expanded determinant.

In the section of Table I for line D, the symbols D_1, D_2 etc. used for the irreducible representations are not to be confused with the D_1 and D_2 defined previously in terms of the radial d functions and their derivatives. It is also to be noted that the vectors ending on line F of Fig. 1. do not actually have the form $K=(k,k,k)$ as indicated in Table I. However, the vectors along the line Λ do have this form and if we continue along this line past the point P we will be considering a line of an adjoining cell which, because of the symmetry of the reciprocal lattice, has the same energy values as the line F. Similarly the line G with $K=(-k+2\pi/a,k,0)$ has the same energy values as the line $K=(2\pi/a,k,k)$ and the plane $K_x=K_y$ has the same energy values as the plane $K_x+K_y=2\pi/a$.

Most of the compatibility relations between the various axes, points and planes have been given by B.S.W. and the reader is referred to their paper for these. We give below some, applicable to our results, which they have omitted.

N_1	N_2	N_3	N_4	N_1'	N_3'	N_4'	P_1	P_3	P_4
G_1	G_3	G_2	G_4	G_4	G_3	G_1	F_1	F_3	F_1F_3
D_1	D_4	D_3	D_2	D_3	D_1	D_4	D_1	D_1D_2	$D_1D_3D_4$
Σ_1	Σ_2	Σ_3	Σ_4	Σ_1	Σ_3	Σ_4			

As an example of how these compatibility relations are to be used, let us consider an energy at which $d_1'=0$. At this energy there will be three bands stuck together at the center of the

TABLE I.—*Continued.*

Lines Λ and F	$K=(k,k,k)$ $T_1=\tan(ka/4)$ $T_2=\tan(ka/2)$ $T_3=\tan(3ka/4)$	
F_1	$1s\ (x+y+z)p\ (xy+xz+yz)d\ xyzf\ \{x(5x^2-3)+y(5y^2-3)+z(5z^2-3)\}f\ \{5(x^4+y^4+z^4)+3\}g$	$16FB_1S_4T_1^2T_2^2T_3^2+T_1^2T_2^2(3D_1S_4+S_2)(3B_3F+B_1)+T_2^2T_3^2(FB_3+3B_1)(D_1S_4+3S_2)+$ $6T_2^2T_1T_3(D_1S_4-S_2)(B_1-FB_3)-24T_2T_1T_3(T_1+T_3)F(B_6S_5+S_6B_5)+16T_1^2T_3^2B_2FS_3$ $+T_1^2(B_2+3B_4F)(S_1+3D_1S_3)+T_3^2(3B_2+FB_4)(3S_1+D_1S_3)+16T_2^2D_1S_2B_3$ $+6T_1T_3(FB_4-B_2)(S_1-D_1S_3)-24T_2(T_1+T_3)D_1(B_6S_5+S_6B_5)+16D_1B_4S_1=0$
$F_3(2)$	$(x-z)p\ (y-z)p\ (yx-yz)d\ (xy-xz)d\ (x^2-y^2)d\ (3z^2-1)d\ \{x(5x^2-3)-z(5z^2-3)\}f$ $\{y(5y^2-3)-z(5z^2-3)\}f$	$T_1^2T_2^2B_1+T_1^2D_2B_2+T_2^2D_1B_3+D_1D_2B_4=0$
Line D	$K=(\pi/a,\pi/a,k)$ $T=\tan(ka/4)$ $C=\mathrm{ctn}(ka/4)$ $T_2=\tan(ka/2)$	
D_1	$1s\ zp\ (3z^2-1)d\ xyd\ z(5z^2-3)f\ xyzf\ \{5(x^4+y^4+z^4)-3\}g$	$12T_2(C-T)(F-D_1)(B_6S_5+B_5S_6)+6T_2^2\{(FB_3-B_1)(S_2-D_1S_4)+2(B_1S_4F+B_3S_2D_1)\}$ $+3T_2^2(T^2+C^2)(B_3F-B_1)(S_2+S_4D_1)-(T^2+C^2)\{2D_2(B_2+FB_4)(S_2+D_1S_4)-(B_2+FB_4)(S_1+D_1S_3)\}$ $-2\{2D_2[(B_2-B_4F)(S_2-S_4D_1)+2(B_2S_4F+B_4S_2D_1)]+(B_2-B_4F)(S_1-S_3D_1)$ $+2(B_2S_3F+B_4S_1D_1)\}=0$
D_2	$(x^2-y^2)d$	$d_2=0$
D_3	$(x+y)p\ (xz+yz)d\ \{x(5x^2-3)+y(5y^2-3)\}f$	$T^2D_1B_3+B_1=0$
D_4	$(x-y)p\ (xz-yz)d\ \{x(5x^2-3)-y(5y^2-3)\}f$	$T^2B_1+D_1B_3=0$
Line G	$K=(-k+2\pi/a,k,0)$ $T=\tan(ka/2)$	
G_1	$1s\ (x-y)p\ xyd\ (3z^2-1)d\ \{x(5x^2-3)-y(5y^2-3)\}f\ \{5(x^4+y^4+z^4)-3\}g$	$T^4B_3\{2D_2(S_2+D_1S_4)+(S_1+D_1S_3)\}+T^4\{B_1(2D_2S_4+S_3)+12B_6D_2S_5+12B_5D_2S_6+3B_4D_2(S_1+D_1S_3)\}$ $+6D_2B_2S_3=0$
G_2	$(xz+yz)d$	$d_1=0$
G_3	$zp\ (xz-yz)d\ z(5z^2-3)f\ xyzf$	$T^2D_1(B_1+FB_4)+2FB_2=0$
G_4	$(x+y)p\ (x^2-y^2)d\ \{x(5x^2-3)+y(5y^2-3)\}f$	$T^2B_1+D_2B_2=0$
Plane $K_x=K_y$	$K=(k,k,u)$ $T=\tan(ka/2)$ $R=\tan(ua/4)$	
—	$(x-y)p\ (xz-yz)d\ (x^2-y^2)d\ \{x(5x^2-3)-y(5y^2-3)\}f$	$T^2R^2B_1+T^2D_1B_3+R^2D_2B_2+D_1D_2B_4=0$
Plane $K_z=0$	$K=(k,u,0)$ $T=\tan[(k+u)a/4]$ $R=\tan[(k-u)a/4]$	
—	$zp\ xzd\ yzd\ z(5z^2-3)f\ xyzf$	$2T^2R^2B_2F+D_1(FB_4+B_2)(T^2+R^2)+2D_1^2B_4=0$

zone and belonging to the representation Γ_{25}'. As we go out along the line Δ two of the bands will continue to stick together, having representation Δ_5 and the third with Δ_2'. Since Δ_5 is compatible with either H_{15} or H_{25}' the two degenerate bands may end at either the energy for which $d_1=0$ or $B_2=0$, and if we assume that the bands we are considering started at an energy lower than any other Δ_5 bands (two more start at energy for which $B_4=0$), they will end at the lower of these two energies, since bands of the same symmetry in general will not intersect, tending to repel each other. Let us consider the energy for $d_1=0$ as the lower. Since this belongs to H_{25}' which is triply degenerate there must be another band ending here, which had the representation Δ_2' (H_{25}' being compatible with $\Delta_2'\Delta_5$). This Δ_2' band may be either the one which started at the same point as the Δ_5 bands (i.e. $d_1'=0$, representation Γ_{25}') or one which started at $f_1=0$ (representation Γ_2'), in which case the former will end at $f_1'=0$ (H_2' also compatible with Δ_2'). The determining factors again are the numerical values and the fact that bands of like symmetry will not cross. Thus if $f_1=0$ occurs at a higher energy than $d_1'=0$, we have the two possibilities shown in Fig. 2. Here we have plotted the energy E (ordinate) as a function of $|K|$. (A) illustrates the case where the energy at which $d_1=0(H_{25}')$ is higher than that at which $f_1'=0(H_2')$. (B) illustrates the reverse case. It must be remembered that the curve Δ_5 represents two bands. In these diagrams the shape of the bands is not significant, the Δ_2' bands and Δ_5 bands may cross (accidental degeneracy) or in the case (B) the Δ_2' band starting at $d_1'=0$ may be above the Δ_5 bands. The correlations between beginnings and ends of bands here are significant, these being the

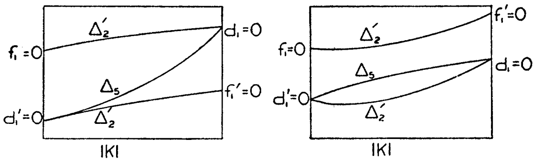

FIG. 2. The plot of energy E as a function of $|K|$. (A) illustrates the case where the energy at which $d_1=0$ is higher than that at which $f_1'=0$. (B) illustrates the reverse case.

only possibilities allowed, assuming $f_1=0$ at higher energy than $d_1'=0$. The possibilities for the opposite case follow in an analogous manner. It must be noted that results obtained here for degeneracies, the various bands which may stick together etc. are not dependent on our approximation. In an exact treatment (i.e., fitting boundary conditions over the whole surface of the cell) while the numerical values would be shifted, the spherical harmonics would still be classified according to representations, the compatibility relations would still hold and all the above results would follow. Thus, for example, the bands arising from a *d* atomic level would still have the same symmetry properties as above (determined essentially by the transformation properties of the various *d* functions). All the information we have obtained about these bands from their symmetry properties would still be valid in an exact treatment, or in any other method of approximation.

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The Zeeman Effect of the Rare Gases

J. B. Green
Mendenhall Laboratory of Physics, Ohio State University, Columbus, Ohio

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The *g* values of the neutral rare gases have been calculated from the atomic coupling factors for the $np^5n'p$ configurations, and excellent agreement is shown to exist between theory and experiment in most cases. From curves of the *g* values, interesting conclusions regarding the the genealogy of the terms in these configurations are noted.

THE Zeeman effect of the neutral rare gases has been studied by a number of investigators, first among them Back[1] who showed, by means of his work on neon, the first discrepancies of the simple Landé theory and its failure to explain the anomalous *g* values that he had observed. At the same time, he gave the first evidence of the *g* sum rule.

A theoretical investigation by Houston[2] led the way to the interpretation of these *g* values and the possibility of their calculation from atomic coupling parameters. Pogany's[1(d), 1(e)] work on the rare gases has shown that excellent agreement exists between theory and experiment for the first excited state of these atoms, the configuration $np^5(n+1)s$, the type of configuration studied by Houston and Condon and Shortley,[3] and Jacquinot[4] has extended the work of Pogany to include the higher series members of this type of configuration in neon, namely the $2p^53s$, $2p^54s$, $2p^55s$, and $2p^56s$ configurations. Although a comparatively large amount of experimental evidence exists, there seem to have been no other calculations made for any other configurations of the rare gases except the $2p^53p$ configuration of neon, where the agreement between theory and experiment is extremely poor.

It is the purpose of the present paper to give a comparison between the observed *g* values and the *g* values calculated from the parameters determined by Bartberger[5] from a least-squares solution of the problem as set up by Shortley[6] for the $np^5n'p$ configurations of the rare gases. Bartberger's parameters were determined from the matrix of the energy set up in *JJ* coupling as the zero-order approximation, but such a zero-order scheme is not suitable for the calculation of *g* values, since the weak-field magnetic interaction terms are not diagonal in *jj* coupling. They are, however, in *LS* coupling, and Bart-

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[1] (a) Back, (neon), Ann. d. Physik **76**, 329 (1925); (b) Terrien and Dykstra, (argon), J. de phys. **5**, 439 (1934); (c) Bakker, (argon, krypton, xenon), Diss. Amsterdam, 1931; (d) Pogany (krypton) Zeits. f. Physik **86**, 729 (1933); (e) Pogany (argon, krypton, xenon) Zeits. f. Physik **93**, 364 (1935).

[2] Houston, Phys. Rev. **33**, 297 (1929).

[3] Condon and Shortley, Phys. Rev. **35**, 1342 (1930); see also Laporte and Inglis, Phys. Rev. **35**, 1337 (1930).

[4] Jacquinot, Comptes rendus **202**, 1578 (1936).

[5] Bartberger, Phys. Rev. **48**, 682 (1935).

[6] Shortley, Phys. Rev. **44**, 666 (1933).