interaction of a particle moving under the action of a nonelectric force,[4] that this scalar may be associated with a scalar potential such as occurs in Nordström's special-relativistic gravitational theory. One sees from (18a) that in applying our theorem to any process in which such an interaction might play a part we must *omit* the matrix elements of this $\mathbf{O}$ in counting the number of factors in the numerator (1) to get n. This is just what is to be expected, since the reason for the alternation of relative signs from order to order in the electric case is to be found in the opposite action of the field on the two signs of charge. The result is of some interest academically, though at present there seems not to be much utility in the concept of a particle which is susceptible both to the action of nonelectric forces and to creation and destruction in pairs.

The operators $\mathbf{O}_4$ and $\mathbf{O}_5$ of (18d) and (18e) cannot be associated with any sort of interaction which has a classical analogue, on account of their unsuitable transformation properties as regards reflection. If, however, an interaction between *two matter-fields* is described by a *biquadratic* form in the Dirac amplitudes, the antisymmetry under reflection can be eliminated by squaring. In fact Wigner, and also Bethe and Bacher,[10] have remarked that these operators, quite as well as the others, can reasonably be used in neutrino theory. It is possible that the symmetry property here described may find applications in this connection.

[10] H. A. Bethe and R. F. Bacher, Rev. Mod. Phys. **8**, 190 (1926).

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Energy Bands for the Face-Centered Lattice

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The Slater method of obtaining wave functions for metallic lattices is applied to the face-centered lattice. The solutions previously obtained by Krutter for this lattice were mainly for certain simple lines in momentum space. Methods are developed for obtaining more general solutions from these special ones. On this basis the entire 110 plane is worked out. For certain new lines in this plane especially simple solutions are given. An approximate method suitable for calculating energy contours in momentum space for small values of momentum is developed.

Introduction

Slater[1] has proposed an extenison of the method of Wigner and Seitz[2] for the calculation of wave functions in the periodic field of metallic lattices. He applied his method to the body-centered lattice with metallic sodium particularly in mind. The method has been applied to lithium[3] (body-centered), to copper[4] (face-centered), and with modifications to diamond[5] and the sodium chloride lattice.[6]

Briefly, the method consists of dividing the lattice into polyhedral cells centered about each atom and containing those points of space nearer that atom than any other atom. The wave function ψ in one of these cells is expanded in terms of surface harmonics times radial functions which are numerical solutions of wave equation. For an atom at a center of symmetry this function is most conveniently handled in the form $\psi=u_g+iu_u$ where u_g is a real even function of the coordinates having the atom as a center (i.e., is expanded in harmonics of even l) and u_u is an odd real function. The functions in other cells are obtained by translating ψ and multiplying it by $e^{i\mathbf{k}\cdot\mathbf{R}}$ where $\mathbf{R}$ is the translation vector. The wave function and its normal derivative are required to be continuous from cell to cell at the midpoints of the cell boundaries.

[1] J. C. Slater, Phys. Rev. **45**, 794 (1934).
[2] Wigner and Seitz, Phys. Rev. **43**, 804 (1933) and **46**, 509 (1934).
[3] J. Millman, Phys. Rev. **47**, 286 (1935); F. Seitz, Phys. Rev. **47**, 400 (1935).
[4] H. M. Krutter, Phys. Rev. **48**, 664 (1935).
[5] George E. Kimball, J. Chem. Phys. **3**, 560 (1935); F. Hund, Physik Zeits. **36**, 888 (1935).
[6] Ewing and Seitz, Phys. Rev. **50**, 760 (1935); W. Shockley, Phys. Rev. **50**, 754 (1935).

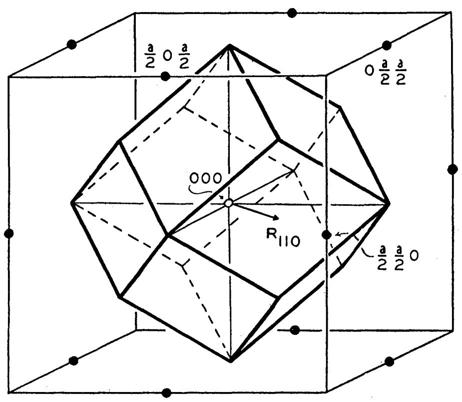


FIG. 1. Cell for the face-centered lattice showing the vector positions of various lattice points and the midpoints of the faces.

For the face-centered lattice, the translations are of the form $a(0\pm\frac{1}{2}\pm\frac{1}{2})$, etc. The polyhedral cell (Fig. 1) is a rhombic dodecahedron whose surfaces are planes bisecting the lines from the origin to the points $a(0\pm\frac{1}{2}\pm\frac{1}{2})$, the midpoints of the faces being $\mathbf{R}_{0\pm1\pm1}=a(0\pm\frac{1}{4}\pm\frac{1}{4})$, etc. Each pair of diametrically opposite midpoints gives rise to two equations of continuity for ψ and the normal derivative ψ' of the form

$$T_{011}u_g-u_u=0, \tag{1}$$

$$u_g'+T_{011}u_u'=0, \tag{2}$$

where $T_{011}=\tan \mathbf{k}\cdot\mathbf{R}_{011}=\tan (k_y+k_z)a/4$. u_g and u_u and their derivatives in respect to increasing r are evaluated at $\mathbf{R}_{011}$. It is convenient to let $\mathbf{k}=(2\pi/a)\boldsymbol{\kappa}$. If $\boldsymbol{\kappa}$ is increased by 111, the $e^{i\mathbf{k}\cdot\mathbf{R}}$ and $\tan \mathbf{k}\cdot\mathbf{R}$ terms are unaltered in value. Hence, our solutions are periodic in $\boldsymbol{\kappa}$-space with the periodicity of a body-centered lattice having $\pm1\pm1\pm1$, ±200, etc., as lattice points. The tangent factors take the simple forms: $T_{011}=\tan \pi(\kappa_y+\kappa_z)/2$, etc.

The six independent directions give twelve conditions and, in order to satisfy them, ψ is expanded in terms of twelve linearly independent functions with arbitrary coefficients. The homogeneous system of equations for these coefficients is then soluble if, and only if, its determinant vanishes. This establishes a functional dependence between $\boldsymbol{\kappa}$ and the energy parameter, which enter through the tangent factors and the values and derivatives of the radial functions, respectively. It is with the nature of this functional relationship that we are concerned.

Krutter has already made a satisfactory choice of the 12 expansion functions. With a modification[7] of notation, these may be listed as in Table I in accordance with their representations in the octahedral group[8] which is the point group for the cell center.

I. SPECIAL DIRECTIONS

No means have been developed for dealing with the determinant for general values of $\boldsymbol{\kappa}$. However, for special directions of $\boldsymbol{\kappa}$ it is possible to get relatively simple expressions. This is a consequence of symmetry of the directions. For the 100 direction, $\boldsymbol{\kappa}=u00$, for example, the functions can be separated into their various symmetry types about the x axis. When this is done, it is found that each type must satisfy the boundary conditions separately and that the satisfying of the conditions on the 110 face, for example, satisfies simultaneously the conditions on the 1–10, 101, 10–1 faces. This reduces the order of the determinantal equations from the 12th to at most the 3rd order for these directions. The corresponding solutions for this line and for 011 and 111 have been published by Krutter and are listed in Table II, along with new solutions developed in this paper.

II. THE 001 PLANE

For values of $\boldsymbol{\kappa}$ lying in certain planes, sufficient symmetry is still preserved to be of considerable help. For $\boldsymbol{\kappa}$ in the 001 plane, that is $\boldsymbol{\kappa}$

TABLE I. *Expansion functions of Krutter.*

	u_g FUNCTIONS
Γ_1	s
Γ_2	$(x^2-y^2)d$, $(y^2-z^2)d$
Γ_5	yzd, zxd, xyd
	u_u FUNCTIONS
Γ_4	xp, yp, zp
Γ_5	$x(y^2-z^2)f$, $y(z^2-x^2)f$, $z(x^2-y^2)f$

[7] Since all the surface harmonics are evaluated for directions such as $0\pm1\pm1$ the factors r^{-l} may conveniently be omitted. x, y, z are then understood to be on the sphere of radius $=\sqrt{2}$. The radial functions s, p, d and f have the customary significance. The ratios s'/s, p'/p, d'/d and f'/f are denoted by σ, π, δ and φ.

[8] For a discussion of the representations of the octahedral group see H. Bethe, Ann. d. Physik **3**, 133 (1929).

of the form $uv0$, it is possible to separate functions into sets which are even and odd with respect to $z\rightarrow -z$. There are only four functions of the odd type, leading to a fourth-order determinant which has been expanded by Krutter and is listed in Table II. The even set appears too complicated to handle in general; however, in addition to the lines 100 and 110 which lie in this plane it is possible to get reduction along the line $\kappa = u10$.

Line I, $\boldsymbol{\kappa}$ = u10 [9]

The simplicity of this line is due to its lying in a 001 plane and a 010 plane simultaneously (Fig. 4a). Hence, it is possible to utilize odd and even classifications for $y\rightarrow -y$ and $z\rightarrow -z$. The results of this classification are shown in Table II.

It is to be noted that Eq. (Ia) is reasonably simple for numerical work, since by virtue of the relation $CT=1$ it is a quadratic in T^2. Thus, for given values of σ, π, δ, and φ, it is possible to solve directly for T and thus find u.

III. The $01\bar{1}$ Plane

For this plane, $\boldsymbol{\kappa} = uvv$, the symmetry in the interchange of y and z is preserved. Hence, the functions can be separated into two sets: odd for interchange of y and z and even. The tangent factors for the dodecahedron are shown in Fig. 2. Only four need be considered, since the two others, $10\bar{1}$ and 110, are related to $1\bar{1}0$ and 101 by interchange of y and z.

Odd set[9]

There are five functions odd in this plane. By the same method as given by Krutter for the odds of 001, we obtain the solution given in Table II.

We shall establish this equation by a different method which we shall use later with the even set. Since the odd functions vanish on 011, the expression cannot involve $K = T_{011}$. Hence, the determinantal equation will be a polynomial in L and M of no higher degree than the second in each term, since each tangent factor occurs in only two of the continuity Eqs. (1) and (2).

Table II. *Classification of the solutions for the face-centered lattice.*[7]

100 direction	$\boldsymbol{\kappa} = u00$	$T_{110} = \tan \pi u/2 = M$
100_a	s, $(2x^2-y^2-z^2)d$, xp	$M^2+3\sigma\delta/\pi(\sigma+2\delta)=0$
100_b	$(y^2-z^2)d$, $x(y^2-z^2)f$	$M^2+\delta/\varphi=0$
100_c	yzd	M arbitrary for $\delta=0$
100_d	xyd, yp, $y(x^2-z^2)f$	$M^2+2\delta/(\pi+\varphi)=0$
100_e	xzd, zp, $z(x^2-z^2)f$	$M^2+2\delta/(\pi+\varphi)=0$
111 direction	$\boldsymbol{\kappa} = uuu$	$T_{011} = \tan \pi u = K$
111_a	s, $(xy+yz+zx)d$, $(x+y+z)p$	$K^2+2\sigma\delta/\pi(\sigma+\delta)=0$
111_b	$[2x^2-y^2-z^2$ $+x(y+z)-2yz]d$, $(2x-y-z)p$, $[y(x^2-z^2)+z(x^2-y^2)]f$	$K^2+4\delta/(\pi+3\varphi)=0$
111_c	$[y^2-z^2+x(y-z)]d$, $(y-z)p$, $[y(x^2-z^2)-z(x^2-y^2)]f$	$K^2+4\delta/(\pi+3\varphi)=0$
111_d	$[2x^2-y^2-z^2$ $-x(y+z)+2yz]d$	K arbitrary for $\delta=0$
111_e	$[y^2-z^2-x(y-z)]d$	K arbitrary for $\delta=0$
111_f	$[x(y^2-z^2)+y(z^2-x^2)$ $+z(x^2-y^2)]f$	K arbitrary for $\varphi=\infty$
011 direction	$\boldsymbol{\kappa} = 0uu$	$T_{011} = K = \tan \pi u$, $T_{101} = L = \tan \pi u/2$
011_a	s, yzd, $(2x^2-y^2-z^2)d$, $(y+z)p$, $[y(x^2-z^2)+z(x^2-y^2)]f$ $2K^2L^2\pi\varphi(5\delta+\sigma)+K^2\delta(\pi+\varphi)(5\sigma+\delta)$ $+4KL\delta(\varphi-\pi)(\sigma-\delta)+2L^2\delta(\pi+\varphi)(\sigma+2\delta)+12\delta^2\sigma=0$	
011_b	$x(y+z)d$, xp	$L^2+\delta/\pi=0$
011_c	$(y^2-z^2)d$, $(y-z)p$, $[y(x^2-z^2)-z(x^2-y^2)]f$	$L^2+2\delta/(\pi+\varphi)=0$
011_d	$x(y-z)d$, $x(y^2-z^2)f$	$L^2+\delta/\varphi=0$
001 plane	$\boldsymbol{\kappa} = uv0$	$T_{101} = \tan \pi u/2$, $T_{011} = \tan \pi v/2$
	xzd, yzd, zp, $z(x^2-y^2)f$ $\left[T^2{}_{101}+\frac{\delta(\pi+\varphi)}{2\pi\varphi}\right]\left[T^2{}_{011}+\frac{\delta(\pi+\varphi)}{2\pi\varphi}\right]=\left[\frac{\delta(\pi-\varphi)}{2\pi\varphi}\right]^2$	
$01\bar{1}$ plane	$\boldsymbol{\kappa} = uvv$	$T_{101} = \tan \pi(u+v)/2$, $T_{1\bar{1}0} = \tan \pi(u-v)/2$
	$(y^2-z^2)d$, $x(y-z)d$, $(y-z)p$, $x(y^2-z^2)f$, $[y(x^2-z^2)-z(x^2-y^2)]f$ $\left[T^2{}_{110}+\frac{\delta(\pi+3\varphi)}{2\varphi(\pi+\varphi)}\right]\left[T^2{}_{101}+\frac{\delta(\pi+3\varphi)}{2\varphi(\pi+\varphi)}\right]=\left[\frac{\delta(\pi-\varphi)}{2\varphi(\pi+\varphi)}\right]^2$	
Line I	$\boldsymbol{\kappa} = u10$	$T_{110} = \tan \pi(u-1)/2 = -\cot \pi u/2 = -C$, $T_{101} = \tan \pi u/2 = T$
I_a	s, $(2x^2-y^2-z^2)d$, $(y^2-z^2)d$, xp, $x(y^2-z^2)f$ $(T^2+C^2)(2\delta+\sigma)(\pi+\varphi)+2(\delta-\sigma)(\varphi-\pi)$ $+2\delta(\delta+2\sigma)+6\pi\varphi=0$	
I_b	xyd, yp, $y(x^2-z^2)f$	$C^2+\delta(\pi+\varphi)/2\pi\varphi=0$
I_c	xzd, zp, $z(x^2-y^2)f$	$T^2+\delta(\pi+\varphi)/2\pi\varphi=0$
I_d	yzd	u arbitrary for $\delta=\infty$

For the even set of the $01\bar{1}$ plane, 311 direction, and Lines II, III, and IV see text.

Furthermore, the symmetry of the problem assures us that if $\boldsymbol{\kappa}_0 = uvv$ is a solution, $-\boldsymbol{\kappa}_0$ must be an equally good solution. Hence, our ex-

[9] This solution was developed independently by the writer and Dr. Krutter. The writer is indebted to Dr. Krutter for a check of his work.

pression must not be altered by replacing κ_0 by $-\kappa_0$. Similarly, replacing κ_0 by $\kappa=-uvv$ and $\kappa=u-v-v$ must leave its value unchanged. This means that the determinant must be invariant under the four (including, of course, identity) symmetry operations in the $01\bar{1}$ plane. If we denote the four operations above by I, R, S, T, we see that determinant D regarded as a function of κ must satisfy the relationship $D=ID=RD=SD=TD$. The transformation scheme of the individual factors is readily found. For example,

$$\begin{aligned} T_{1\bar{1}0}&=\tan \pi(u-v)/2=M,\\ RM&=\tan \pi(-u+v)/2=-M,\\ SM&=\tan \pi(-u-v)/2=-L,\\ TM&=\tan \pi(u+v)/2=L. \end{aligned}$$

This is expressed in tabular form in Table III. From this it is possible to list the allowable terms which may occur in D. For example, if L^bM^c occurs, it must be present in a combination with L^cM^b that is unaltered by the operations R, S and T. From the group property of I, R, S, T, it may easily be verified that the only such form is $(I+R+S+T)L^bM^c=[1+(-1)^{b+c}][L^bM^c+L^cM^b]$. Hence, the most general form of D will be, except for a factor independent of L and M, $D=A+BLM+C(L^2+M^2)+L^2M^2$. It is now possible to evaluate the constants, A, B and C, from the solutions in special directions.

100 direction

For this $M=L$ and $D=0$ reduces to $D=A+(B+2C)M^2+M^4=0$. This must factor into $100b$ and $100d$ ($100d-100e$ is odd in the $01\bar{1}$ plane and has the same equation as $100d$ and $100e$); the two known solutions for the odd functions. Hence, D must contain $M^2+\delta/\varphi$ and $M^2+2\delta/(\pi+\varphi)$ as factors. Therefore,

$$\begin{aligned} A&=2\delta^2/\varphi(\pi+\varphi),\\ B+2C&=\delta(\pi+3\varphi)/\varphi(\pi+\varphi). \end{aligned}$$

011 direction

For this $M=-L$ and $D=0$ becomes $D=A+(-B+2C)L^2+L^4=0$. The known solutions $110c$ and $110d$ are the same as $100b$ and $100d$. Hence, $B=0$, and

$$D=2\delta^2/\varphi(\pi+\varphi)+[\delta(\pi+3\varphi)/2\varphi(\pi+\varphi)][L^2+M^2]+L^2M^2=0.$$

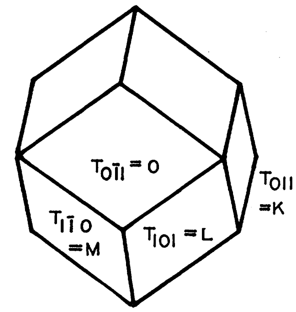


FIG. 2. Cell for the face-centered lattice showing the values of the tangent factors for $\kappa=uvv$ (the $01\bar{1}$ plane).

This is equivalent to the solution in Table II.

Even set

The procedure of the odd set can be carried out for the even set also. For this set we expect to get terms in K as well as L and M. The allowed form is given below. Since only the ratios of the coefficients can be found by this method, the coefficient of the zeroth order term has been made unity.

$$\begin{aligned} D=1&+[BK(L-M)+CLM+DK^2\\ &+E(L^2+M^2)]+[FK^2LM+GK^2(L^2+M^2)\\ &+HKLM(L-M)+JL^2M^2]+PK^2L^2M^2. \end{aligned}$$

100 direction

For this line $K=0$, $L=M$, and

$$D=1+[C+2E]M^2+JM^4=0.$$

From Table II we see that this must have the factors $M^2+3\sigma\delta/\pi(2\delta+\sigma)$ and $M^2+2\delta/(\pi+\varphi)$. Equating the ratios of coefficients, we get

$$C+2E=\frac{(5\sigma\pi+4\delta\pi+3\sigma\varphi)}{6\sigma\delta},$$

$$J=\frac{\pi(\pi+\varphi)(2\delta+\sigma)}{6\sigma\delta^2}.$$

011 direction

For this $M=-L$ and $|M|\neq|K|\neq 0$ and

$$\begin{aligned} D=1&+2BKL+(-C+2E)L^2\\ &+DK^2+(-F+2G)K^2L^2\\ &-2HKL^3+JL^4+PK^2L^4=0. \end{aligned}$$

Proceeding as above, we find that the factors are $011a$ and $011b$ and that the coefficients are

$$B=\frac{(\varphi-\pi)(\sigma-\delta)}{6\sigma\delta},$$

$$-C+2E=\frac{(\pi+\varphi)(2\delta+\sigma)+6\sigma\pi}{6\sigma\delta},$$

$$D=\frac{(\pi+\varphi)(\delta+5\sigma)}{12\sigma\delta},$$

$$-F+2G=\frac{\pi[2\varphi(5\delta+\sigma)+(\pi+\varphi)(\delta+5\sigma)]}{12\sigma\delta^2},$$

$$H=\frac{\pi(\pi-\varphi)(\sigma-\delta)}{6\sigma\delta^2},$$

$$J=\frac{\pi(\pi+\varphi)(2\delta+\sigma)}{6\sigma\delta^2},$$

$$P=\frac{\pi^2\varphi(5\delta+\sigma)}{6\sigma\delta^3}.$$

111 direction. $M=0$, $K=L$

$$D=1+(B+D+E)K^2+GK^4=0.$$

The known solutions are $111a$ and $111b$ and the results are

$$B+D+E=\frac{3\sigma\pi+3\sigma\varphi+2\delta\pi}{4\sigma\delta},$$

$$G=\frac{\pi(\pi+3\varphi)(\sigma+\delta)}{8\sigma\delta^2}.$$

TABLE III. *Transformation scheme for the tangent factors of the 011 plane.*

I	R	S	T
uvv	$-u-v-v$	$-uvv$	$u-v-v$
K	$-K$	K	$-K$
L	$-L$	$-M$	M
M	$-M$	$-L$	L

TABLE IV.

COEFFICIENT	TERM
$B=(\varphi-\pi)(\sigma-\delta)/6\sigma\delta$	$K(L-M)$
$C=(\varphi-\pi)(\sigma-\delta)/6\sigma\delta$	LM
$D=(\pi+\varphi)(\delta+5\sigma)/12\sigma\delta$	K^2
$E=(3\pi+\varphi)(2\sigma+\delta)/12\sigma\delta$	L^2+M^2
$F=\pi(\pi-\varphi)(\delta-\sigma)/6\sigma\delta^2$	K^2LM
$G=\pi(\pi+3\varphi)(\sigma+\delta)/8\sigma\delta^2$	$K^2(L^2+M^2)$
$H=\pi(\pi-\varphi)(\sigma-\delta)/6\sigma\delta^2$	$KLM(L-M)$
$J=\pi(\pi+\varphi)(2\delta+\sigma)/6\sigma\delta^2$	L^2M^2
$P=\pi^2\varphi(5\delta+\sigma)/6\sigma\delta^3$	$K^2L^2M^2$

From these three lines we thus get 11 equations for the 9 coefficients of D. From them we can determine all the coefficients and have two extra equations as a check. The results are given in Table IV.

IV. SPECIAL LINES IN THE $01\bar{1}$ PLANE

For certain lines in the $01\bar{1}$ plane, D takes a specially simple form.

311 direction

For the 311 direction, $\boldsymbol{\kappa}=3v, v, v$ and $K=M=\tan(\pi v)$ and $L=\tan(2\pi v)$. Hence, there are only two distinct tangent factors in D. Such expressions as this result and $011a$ can best be used in calculation by making a table of the values of the terms such as K^2, K^2L^2, etc., which occur in them. Then for a fixed value of the energy, D is evaluated as a function of v and the zeros are found.

Line II. $\boldsymbol{\kappa}=u\frac{1}{2}\frac{1}{2}$

$K=\infty$, $L=\tan\pi(u+\frac{1}{2})/2=-\cot\pi(u-\frac{1}{2})/2=-C$, $M=\tan\pi(u-\frac{1}{2})/2=T$. For this we must equate the coefficients of K^2 to zero, obtaining

$$(C^2+T^2)G+(D-F+P)=0.$$

which, as a consequence of $CT=1$, is a quadratic in C^2 as is solution Ia.

Line III. $\boldsymbol{\kappa}=(1-v), v, v$

$K=\tan\ \pi v=T$, $L=\infty$, $M=-\cot\ \pi v=-C$. For this we must equate the coefficient of L^2 to zero, obtaining

$$GT^2+JC^2+(E+H+P)=0.$$

This is again a quadratic in C^2.

V. THE CASE OF $\kappa\ll 1$

From an inspection of D it can be seen that when $\boldsymbol{\kappa}\to 0$ either σ or $\delta\to 0$ or π or $\varphi\to\infty$.[10] It can also be seen that for a given small value of $\boldsymbol{\kappa}$, the equation becomes linear in σ for $\sigma\to 0$; cubic in δ; quadratic in π; and linear in φ. This is a consequence of the fact that one s function, three d functions, two p functions and one f function compose the even set of the $01\bar{1}$ plane.

[10] The pathological case of several of these requirements being met at once will not be considered.

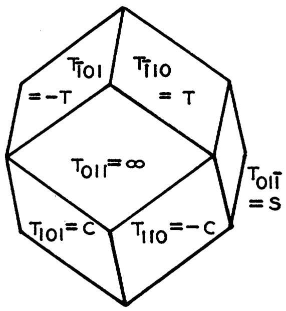


FIG. 3. Cell for the face-centered lattice showing the values of the tangent factors for $\boldsymbol{\kappa} = u(01\bar{1}) + \frac{1}{2}(111)$, line IV. $T = \tan \pi u/2$, $C = \cot \pi u/2$, $S = \tan \pi u$.

If $\boldsymbol{\kappa}$ is small enough, it is possible to expand K, L and M in powers of u and v. It is more convenient to use symmetry arguments, however, in order to establish the form of the result and then evaluate the unknown coefficients from special directions. For example, the result for $\sigma \to 0$ must be

$$\sigma + au^2 + bv^2 = 0.$$

From the 100 condition, we see that

$$-\sigma = 2p'M^2/3p \doteq (p'\pi^2/6p)u^2 \doteq au^2$$

(here π has its conventional meaning and does not denote p'/p) and from 111,

$$-\sigma = 2p'K^2/p \doteq (p'\pi^2/2p)u^2 \doteq (a+b)u^2.$$

Hence, $2a = b = \pi^2 p'/3p$, and the σ contour is a circle.[11]

For the p functions, the form must be

$$(p/p')^2 + (p/p')(au^2 + bv^2) + (cu^4 + du^2v^2 + ev^4) = 0.$$

The coefficients of this form can be evaluated from the 100, 011 and 111 directions.

A similar process or else direct expansion of D can be used for the d functions; and the same methods are applicable to the 001 plane or to general space directions.

For all the cases we shall find that for a given direction of $\boldsymbol{\kappa}$ the values of σ and the values of $1/\pi$ will be linear functions of $|\boldsymbol{\kappa}|^2$. For $|\sigma|$ and $|1/\pi| \ll 1$, these quantities will be approximately linear functions of the energy. Hence the energy *versus* $\boldsymbol{\kappa}$ curves will be single (for s), double (for p), etc., parabolas in $\boldsymbol{\kappa}$.

[11] This can also be seen from the more general statement that for the three-dimensional case of $|\kappa| \ll 1$ the cubic symmetry requires $\sigma + a(\kappa_x^2 + \kappa_y^2 + \kappa_z^2) = 0$, the equation of a sphere.

VI. LINE IV. $\kappa = u(01\bar{1}) + \frac{1}{2}(111)$

For functions of the form $\psi = u_g + iu_u$ for which $\boldsymbol{\kappa} = u(01\bar{1}) + \frac{1}{2}(111)$, it is possible to split the set of 12 functions into smaller sets of 5 and 7. Consider the function $A\psi$ obtained from ψ by interchanging y and z; it will satisfy the same continuity requirements as ψ save that its $\boldsymbol{\kappa}$ will be $A\boldsymbol{\kappa} = u(0\bar{1}1) + \frac{1}{2}(111) = -\boldsymbol{\kappa} + 111$. Due to the periodicity of $\boldsymbol{\kappa}$-space, $-\boldsymbol{\kappa} + 111$ is equivalent to $-\boldsymbol{\kappa}$. Now the complex conjugate ψ^* of ψ will clearly correspond to $-\boldsymbol{\kappa}$. We can now introduce an operator $P = (A)^*$ which operating on ψ leaves its $\boldsymbol{\kappa}$ value invariant and also its energy value (since both A and $*$ do). Since P is its own reciprocal, we can conclude from the representation theory of groups (or from considerations of $(\psi + P\psi)$ and $(\psi - P\psi)$) that we can classify the functions into two sets according to whether $P\psi = \psi$ or $-\psi$.

Set 1

For $P\psi = \psi$ we find that $Au_g = u_g$ and $Au_u = -u_u$ so that we should use even harmonics which are even in yz interchange and odd harmonics which are odd. This gives the set of functions:

$$s,\quad x(y+z)d,\quad yzd,\quad (2x^2-y^2-z^2)d,\quad (y-z)p,$$
$$x(y^2-z^2)f,\quad [y(x^2-z^2) - z(x^2-y^2)]f.$$

Set 2

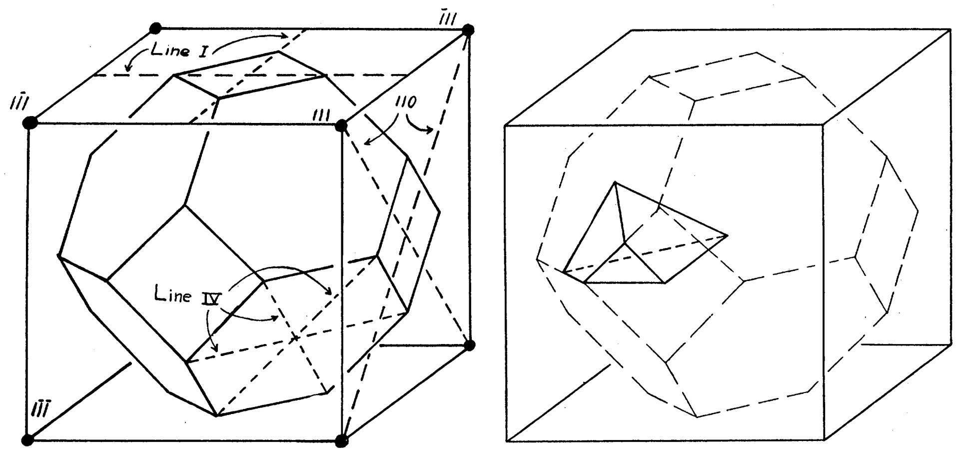
From $P\psi = -\psi$ we find $Au_g = -u_g$ and $Au_u = u_u$ so that even harmonics should be odd for yz interchange; odd harmonics, even. The functions of this set are:

$$x(y-z)d,\quad (y^2-z^2)d,\quad xp,\quad (y+z)p,$$
$$[y(x^2-z^2) + z(x^2-y^2)]f.$$

The scheme of the tangent factors is shown in the Fig. 3. $\bar{1}01$ and 110 are equivalent to $\bar{1}10$ and 101, respectively, by the P symmetry. The 011 face gives only one condition on each set, since for set 1 the u_u functions automatically vanish there as do the u_g of set 2. Due to its complexity, set 1 has not been worked out. The seventh-order determinant to which it leads can be easily set up, but the expansion is tedious.

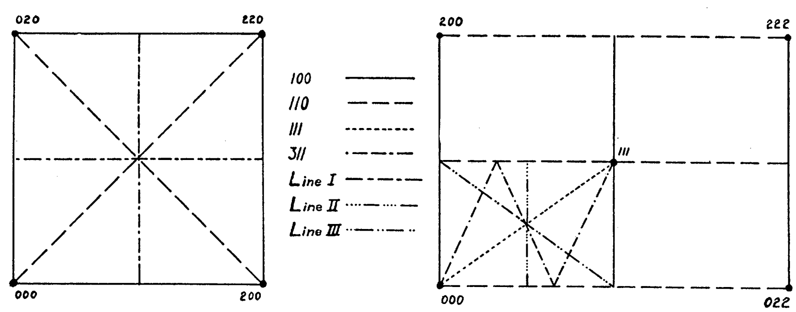
Expansion of set 2

Set 2 is simpler, since all of its functions vanish on $01\bar{1}$, thus leading to only five conditions for the coefficients. The resultant determinantal



(a) (b)

FIG. 4. Views of body-centered $\boldsymbol{\kappa}$-space. *a*. $\boldsymbol{\kappa}$ lattice and first Brillouin zone showing the various solutions. *b*. Fundamental segment of the first zone.



(c) (d)

FIG. 4. *c*. 001 plane, showing the solutions. *d*. $01\bar{1}$ plane, showing the solutions. Only one-quarter of the diagram is completed; the remainder follows from symmetry.

equation may be reduced to

$$(C^2+T^2)\delta\pi(3+\pi/\varphi)+2[\delta^2(1+\pi/\varphi)+2\pi^2]=0.$$

This can be treated by the same method as was used for line Ia.

Summary and Final Remarks

Fig. 4*a* shows the first Brillouin zone in body-centered $\boldsymbol{\kappa}$-space. Fig. 4*b* shows the fundamental segment of the zone which contains all representative points. Any point outside the segment is equivalent to some point of the segment by the symmetry of the lattice. The solutions for the 001 and $01\bar{1}$ planes are indicated in 4*c* and 4*d*. Four of the five faces of the fundamental segment are of 001 or 011 type, and the fifth contains line IV which is a line of symmetry for this face. Hence the energy contours may be considered as well known on the surface of the segment. When this information is combined with that obtained for $|\boldsymbol{\kappa}|\ll 1$ and the symmetry conditions required by reflection planes in the $\boldsymbol{\kappa}$ lattice, it should be possible to draw fairly accurate space contours in $\boldsymbol{\kappa}$-space.[12]

An attempt to apply the methods used for the even functions of the $01\bar{1}$ plane to the even functions of the 001 plane has been made. It is found that there are more coefficients to be determined than can be evaluated from the known solutions of 100, 110, and line I. The remaining coefficients could be evaluated by partial expansion of the eighth-order determinant for the plane.

[12] Some space contours drawn according to this scheme have been published by the writer. Phys. Rev. **50**, 754 (1936).