

A CONSTANT POTENTIAL METHOD  
FOR ENERGY BANDS IN SOLIDS

by

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1958



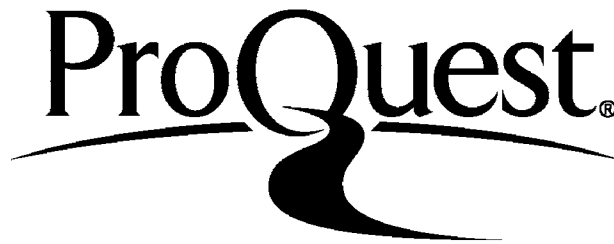
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ABSTRACT

The constant potential method assumes that the effective potential is spherically symmetrical within the inscribed spheres of the atomic polyhedra and constant in the space between them . The variation principle giving the energy levels of electrons in monoatomic lattices is expressed here as a surface integral over the boundary of the volume. Once certain " structure constants " appearing in this method have been calculated for a given type of lattice , they may be used with different potentials without much additional effort . This method has been tested with the empty lattice test for  $k=0$  ( Al type lattice ) and has further been applied to the monoatomic substance ( Al ). The results of some calculations have been reported in both cases .

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## INTRODUCTION

In the last decade , a number of attempts at a theoretical determination of wave functions and energy levels of electrons in solids have demonstrated clearly that the amount of labour involved in such a study is enormous. The discovery of a procedure which enables us to make short - cuts in the calculations without destroying the resonableness of the model must therefore be of interest .

The present paper is concerned with the presentation of such a procedure . Among others, Kohn, Rostoker have recently proposed a similar method based on a variational procedure derived from an integral equation for the Bloch function . This method also assumes that the lattice potential is spherically symmetric about each ion core within a sphere inscribed in the atomic cell, and is constant in the volume outside that sphere. The calculation of the band structure for a particular ion potential requires only the knowledge of the logarithmic derivative of the radial wave functions of different

$l$  ( azimuthal quantum number ) on the surface of this sphere . It is essentially a variation of the Wigner - Seitz cellular method . In principle , this method can be used for any substance . Moreover , once certain "structure constants" appearing in the method have been calculated for a given type of lattice , they may be used with different potentials ( corresponding to other substances ) without much additional effort . Dr.L.Pincherle has even successfully applied a similar procedure to the diatomic substance  $PbS$ .

To obtain a critical evaluation of the rigour of this method in the derivation of energy levels it was applied to a case in which the exact solution is known , namely to an artificial crystal in which the potential is zero throughout its volume ( empty lattice test ). It may be of some interest to consider whether this procedure is applicable to the same extent as with other methods, therefore we have applied it to the well known aluminium crystal which

has a high density of conduction electrons and whose ion core is relatively small.

I have a great pleasure in expressing my real gratitude to Dr. L. Pincherle for his invaluable guidance and encouragement throughout this work.

THE CELLULAR METHOD

We shall not be wrong to assume that the most highly developed and widely applied technique for obtaining one electron wave functions in solids is the cellular method. The Schrodinger problem in the crystal may be reduced to a single cell of the space lattice by the use of the Bloch form for the wave function. When applying the cellular method, the shape of the cells into which we divide the crystal is arbitrary. In the case of a simple monoatomic solid for which all the atoms are translationally equivalent, the unit cell chosen may be polyhedron of smallest volume, ( Wigner - Seitz cell ) whose plane faces bisect orthogonally the lines joining the atom to its neighbours.

The basic assumption of the method is that the ion core wave functions remain essentially unchanged in going from the free atom to the solid, the valence wave functions, however, must be solutions of a self-consistent field calculation in the crystal. Thus we may



expand the wave function ' $\psi_K$ ' in terms of orthogonal functions appropriate to the central field , the expansion being only valid inside the W - S cell . However, the wave function can be extended to the neighbouring polyhedra , joining the individual solutions at the boundary by means of the continuity requirement on wave function and normal derivative together with the Bloch condition ( eq. 3 and 4 page 19 ). One of the drastic approximations of the cellular method is to assume , within each cell , a spherically symmetrical potential , so that the wave function should be able to expand in spherical harmonics about the centrally located atomic nucleus . When we reach the outer part of each cell the approximation becomes still poorer . It is also prone to produce discontinuities in the potential at the boundaries of the cells , though these may not be very relevant . In order to reduce the cellular method to a practical scheme , boundary conditions are applied at selected points on the polyhedron surface. Hence equation '1' can be satisfied at a relatively

small number of points only . The boundary conditions can also be applied as area conditions. In this case , the functions and normal derivatives appearing in eq. 3 and 4 ( page 19 ) may be replaced by averages over the appropriate areas . In the point matching procedure considerable care must be taken in choosing the points at which the boundary conditions are applied . One of the method used for testing the suitability of arbitrarily chosen boundary points is the empty lattice test ( described later on ). It will be convenient to use the unnormalised Kubic Harmonics absorbing the normalisation into the lattice constants . An adequate number of boundary conditions leads to simultaneous equations which are compatible only if the determinant of the lattice coefficients vanishes . This will occur only with certain discrete energies .

In order to utilize fully the symmetry of the crystal , it is customary to express the wave function in the form

$$\psi_{\kappa} = \sum_{\ell t} C_{\ell t} K_{\ell t}(\theta \varphi) \psi_{\ell}(\gamma E_{\kappa})/r \quad (1)$$

' $K_{\ell t}$ ' is a lattice harmonic, that is to say a linear combination of spherical harmonics chosen to transform the wave function according to one of the irreducible representations of the group of the wave vector ' $K$ '. The wave functions associated with the point ' $K$ ' fall into orthogonal sets, each set having a particular type of symmetry of its own. The type differs for each irreducible representation of the group of ' $K$ '. The azimuthal quantum number is ' $\ell$ '. The index ' $t$ ' indicates that more than one ' $K$ ' may be derived from spherical harmonics of the order ' $\ell$ '. The coefficients ' $C_{\ell t}$ ' may be determined by boundary conditions which require the wave functions of the neighbouring atom to fit together smoothly enough at cell surface.

The angular functions used in a cubic crystal have been termed "Kubic Harmonics". For a small ' $\ell$ ', the K.H. of the lowest order are simply surface harmonics. For ' $\ell > 3$ ', however, Van der Lage and Bethe have devised another method. Intending to construct

a set of functions which would be satisfactory in two conditions, they proceeded by first constructing a set of functions apt to satisfy the first condition, and subsequently modifying these functions without affecting their conformity to this condition, so that they satisfy the second condition as well. Thus K.H. must satisfy two conditions a) they must have correct symmetry b) they must be the solution of Legendre's differential equation. The first step consists in constructing symmetrically correct polynomials ( C.P. ) of order ' $l$ ' which are, moreover, linearly independent of each other, and then it is only necessary to make ' $\frac{C.P.}{r^l}$ ' orthogonal to the K.H. of the same type and lower ' $l$ '.

Any set of linearly independent degenerate wave functions must, under the operation of the group of the wave equation, transform by an irreducible representation of this group. As to the crystal, its relevant group is the space group of the crystal. There are two types of restriction on possible wave

functions :

a) translational restriction

b) rotational restriction

The rotation group is the full group of rotations about a point in space in three dimensions, but the effect of rotational symmetry on possible wave functions is modified when only certain exclusive rotations are admissible. The result can be then expressed as the direct sum of the irreducible representation of the subgroups.

The symmetry of translation results in two effects: first, each atomic level becomes a band of levels - as many levels as there are atoms, each of the levels corresponding to a different value of ' $k$ '; secondly, each value of ' $k$ ' is correlated with a particular rotation group on whose representations the wave functions depend. It is sufficient to consider the symmetry properties of the wave function belonging to a ' $k$ ' whose operational group belongs to the cubic group type where ' $k$ ' is left invariant. This group ,



comprising namely subgroups of rotation, is larger than a unit element. The rotation symmetry of other wave functions becomes automatically satisfactory when  $\psi_k = u e^{i k r}$ . Hence the reduction of the original representation need only be studied when it can be regarded as a representation of a subgroup of rotation of the kind where 'k' is left invariant, and not of the whole rotation group.

In practice, only 'k' of a fairly high degree of symmetry need be considered. If the symmetry of 'k' is low, the method provides no more than a small number of coefficients: 'C<sub>kt</sub>'.

For the 'Al' group of substances the potential in the lattice has a face centred cubic symmetry, and so has the Hamiltonian. Since the simplest form of the B.Z. ( page 13 ) consists of eight equal hexagons and six equal squares - a truncated octahedron - it is not unexceptionally fixed by this symmetry. The reciprocal lattice in question has the

same symmetry as the cube or the octahedron . Thus  
the group of  $k(0.0.0)$  is a full cubic group  
and its irreducible representations , each with a  
corresponding type of wave function , are denoted by  $\Gamma$

THE BRILLOUIN ZONE

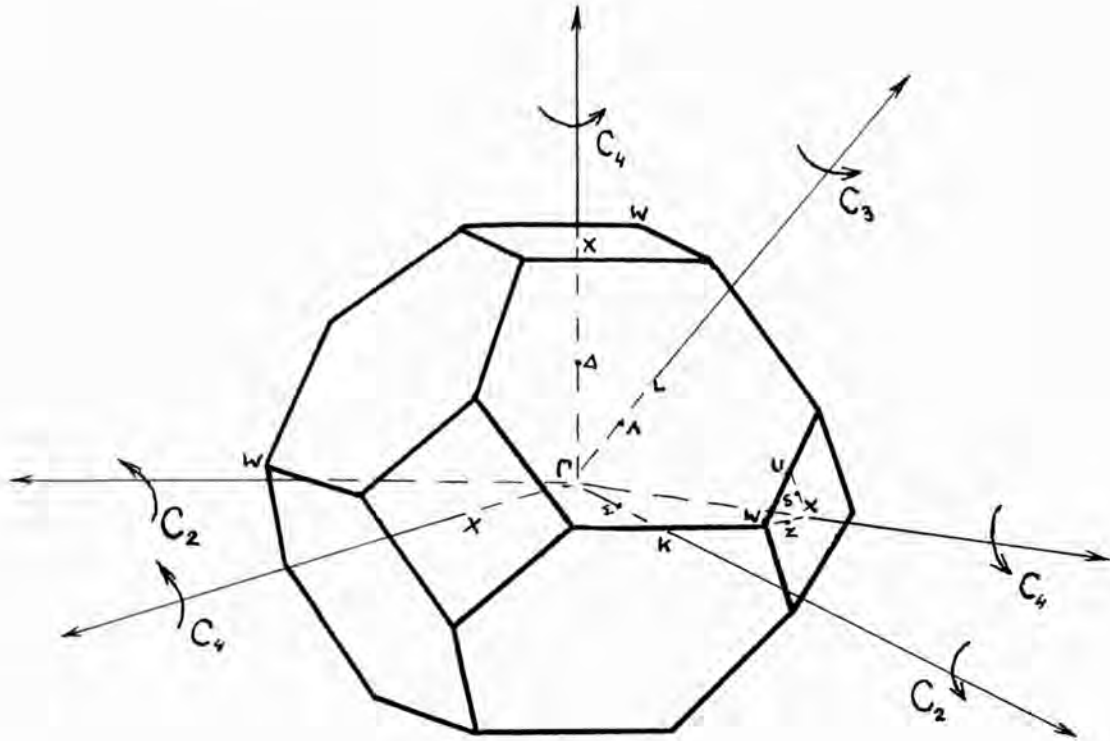


Fig. 1

The first Brillouin zone of a face - centred cubic crystal . Letters indicate points associated with wave functions of particular symmetries .  $C_n$  is the axis of rotation where index  $n$  means  $n$  - folded axis .



WIGNER - SEITZ LATTICE

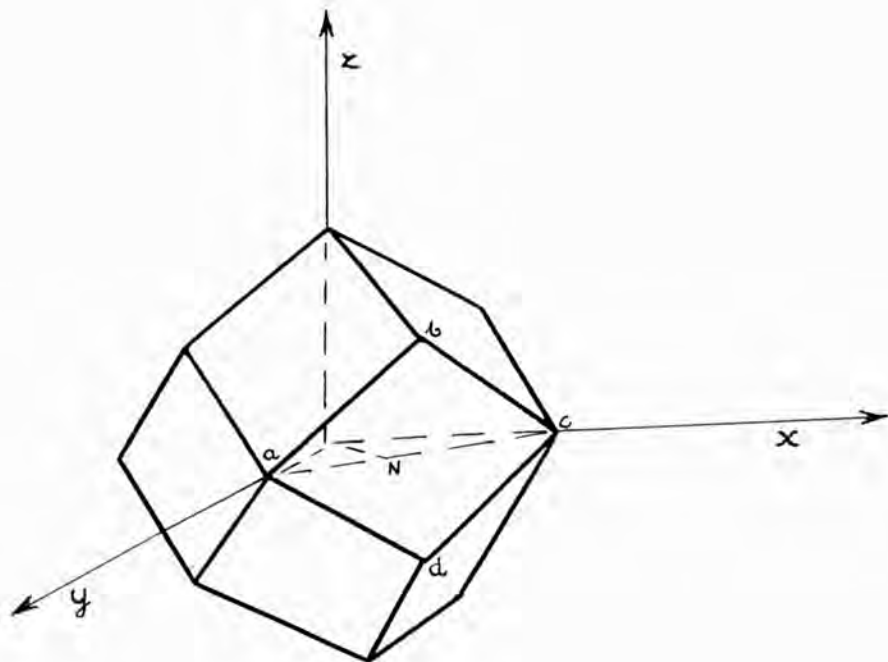


Fig. 2

Wigner - Seitz lattice of a face centred cubic crystal .

VARIATIONAL PROCEDURE  
FOR SATISFYING BOUNDARY CONDITIONS

The whole problem of calculation  $E(k)$  is greatly simplified when the effective potential is spherically symmetrical within the inscribed spheres of the atomic polyhedra and constant in the space between them . As has been pointed out in the introduction , the overwhelming part of the work of calculating the energy bands consists in the calculation of certain geometrical " structure constants " ( in this case , of the structure constants of substance like Al ) which must be calculated a priori, once and for all , for each type of lattice . These apart , the only other information required consists in the logarithmic derivatives ,  $\frac{\partial R_l}{\partial r} / R_l$  at the surface of the inscribed sphere of s. p. d. .... solutions of the Schrodinger equation with the given  $V(r)$  . As will be shown in further calculations , these can be obtained by numerical integration or

directly from the atomic spectra without the explicit introduction of  $V(r)$  .

Then the functions  $R_l(Er)$  may be considered to form a one parameter family ( parameter E ) of these solutions of eq. 15 which are zero at origin. In terms of these, a new function  $\phi_{r_0}^l(E)$  may be defined as the logarithmic derivative of  $R_l(Er)$

at  $r=r_0$  by

$$\phi_{r_0}^l(E) = \left\{ \frac{1}{R_l(Er)} \frac{dR_l(Er)}{dr} \right\}_{r=r_0}$$

It can be shown quite generally that for sufficiently small values of  $r_0$ ,  $\phi_{r_0}^l(E)$  is a smooth, non - oscillating function of E. For since the function  $V(r)$  must be expressible in  $Ry$  units in the form  $-\frac{2Z}{r} + q(r)$ , where  $q(r)$  is an analytic function with a zero at origin, it follows that the logarithmic derivative can always be expressed in the form

$$\phi_{r_0}^l(E) = \frac{1}{R} + \sum_{k=0}^{\infty} a_k^l(E) r_0^k$$

in which the coefficients  $a_k^l$  are polynomial functions

of the energy  $E$  . Further , the degree of these polynomial functions increases quite slowly with  $k$  ;  $a_0^l$  is independent of  $E$ ,  $a_1^l$  and  $a_2^l$  are linear functions of  $E$  , and generally  $a_{2k-1}^l$  and  $a_{2k}^l$  are polynomials of degree  $k$  in  $E$  . Thus , for all physically significant values of  $E$  and for sufficiently small values of  $\gamma_0$  ,  $\phi_{\gamma_0}^l(E)$  will be constant , since terms beyond  $a_0^l$  may be discarded . With  $\gamma_0$  somewhat larger , so that the coefficients  $a_3^l$  must be kept ,  $\phi_{\gamma_0}^l(E)$  will show a linear dependence on  $E$  . For a given value of  $E$  the solutions  $R_l(E\gamma)$  of the wave equation which is zero at the origin must be identical ( in the hydrogenic region  $\gamma \gg \gamma_0$  ) with some linear combination of Whittaker' s two functions . The particular linear combination desired is completely determined by the function  $\phi_{\gamma_0}^l(E)$  , which is the logarithmic derivative of the correct solution ,  $R_l(\gamma E)$  computed at  $\gamma_0$  . If the hydrogenic region extends near enough the core so that  $\phi_{\gamma_0}^l(E)$  is a well-behaved function of  $E$  , then the behaviour of  $\phi_{\gamma_0}^l(E)$  is completely determined by the first few

values of  $\phi_{\gamma_0}^l(E_\kappa)$ , where the  $E_\kappa$  are the atomic term levels .

In practice it is necessary to choose the largest matching radius  $\gamma_0$  such that the points  $\phi_{\gamma_0}^l(E_\kappa)$  lie on a curve which may be described by a simple polynomial .

It should be emphasised that , in spite of the assumption of a spherical  $V(r)$  , this method is not equivalent to the spherical approximation of Wigner and Seitz , for the polyhedron , which is approximated by a sphere by Wigner and Seitz , is here exactly taken into account on its actual shape .

We shall proceed now to state the boundary value problem which we wish to formulate as a variational principle

$$\left[ -\nabla^2 + V(r) - E \right] \psi(r) = 0 \quad (2)$$

for all  $r$  inside the polyhedron .

Every boundary point  $r$  corresponds to a conjugate point  $r'$ , also on the boundary, in such a way that  $r'-r$  becomes one of the fundamental translation vectors  $\tau_r$ . It will be seen that, in this particular case  $\tau_r$  is constant on each face and that  $\tau_{r'} = -\tau_r$

$$\psi(r') = \exp(ik\tau_r)\psi(r) \quad (3)$$

for all  $r$  on the surface of the polyhedron.

$$\frac{\partial\psi(r')}{\partial n} = -\exp(ik\tau_r)\frac{\partial\psi(r)}{\partial n} \quad (4)$$

Here,  $k$  is the wave vector and  $\frac{\partial}{\partial n}$  denotes the differentiation along the outward normal at the point in question. The minus sign in 4 is here to indicate that the outward normals at  $r$  and  $r'$  are opposite in direction.

To obtain an equivalent variational principle, we consider the functional

$$I = \int_{\Omega} \psi^* [-\nabla^2 + V(r) - E] \psi d\omega \quad (5)$$

where  $\Omega$  denotes the interior of the polyhedron. The first variation can be represented as an integral over the bounding surface  $S$  of the polyhedron :

$$dI = \int_S \left( \delta\psi \frac{\partial}{\partial n} \psi^* - \psi^* \frac{\partial}{\partial n} \delta\psi \right) ds \quad (6)$$

considering the first term of the real part of 6 , we undertake the following transformation :

$$\begin{aligned} \operatorname{Re} \int_S \delta\psi(r) \frac{\partial}{\partial n} \psi^*(r) ds &= \operatorname{Re} \int_S \frac{\partial}{\partial n} \psi(r) \delta\psi^*(r) ds \\ &= \operatorname{Re} \int_S \frac{\partial}{\partial n} \psi(r) \delta\psi^*(r) ds \\ &= \operatorname{Re} \int_S -\frac{\partial}{\partial n} \delta\psi(r) \psi^*(r) \exp(ikr_r) ds \quad (7) \end{aligned}$$

where the last step refers to the boundary condition. The second term of 6 can , in virtue of 3 , be represented as

$$\begin{aligned} \operatorname{Re} \int_S -\frac{\partial}{\partial n} \delta\psi(r) \psi^*(r) ds &= \\ &= \operatorname{Re} \int_S -\frac{\partial}{\partial n} \delta\psi(r) \psi(r) \exp(ikr_r) ds \quad (8) \end{aligned}$$



Combining these two results we obtain

$$\delta(\text{Re}I) = -\delta \left[ \text{Re} \int_S \frac{\partial}{\partial n} \psi(r) \psi^*(r) \exp(ikr_r) ds \right] \quad (9)$$

The desired variational principle can now be expressed in the following form :

$$\begin{aligned} \mathcal{J}(\psi, k, E) = & \text{Re} \left[ \int_{\Omega} \psi^* (-\nabla^2 + V - E) \psi d\omega + \right. \\ & \left. + \int_S \frac{\partial \psi(r)}{\partial n} \psi^*(r) \exp(ikr_r) ds \right] = \\ & = \text{stationary} \quad (10) \end{aligned}$$

Obviously, the functional  $\mathcal{J}$  will vanish for the correct  $\psi$ ,  $k$  and  $E$ . We may also note two special forms of 10. If the admitted trial functions all satisfy the boundary conditions, we obtain

$$I_1 = \int_{\Omega} \psi^* (-\nabla^2 + V - E) \psi d\omega = \text{stationary} \quad (11)$$

if, however, the trial functions (as is the case here), satisfy the wave equation 2, we obtain

$$I_2 = \text{Re} \int_S \frac{\partial \psi(r)}{\partial n} \psi^*(r) \exp(ikr_r) ds = \quad (12)$$

= stationary



In the case of  $k=0$  ( this particular case )  $I_2$   
reduces:

to 
$$\operatorname{Re} \int_S \frac{\partial \psi(r)}{\partial n} \psi^*(r) ds \quad (13)$$

A NEW FORM OF CONSTANT POTENTIAL METHOD

The general form of wave function to be used

$$\text{is } \psi_{\kappa} = \sum_{\ell t} C_{\ell t}(\kappa) K_{\ell t}(\kappa, \theta, \varphi) R_{\ell}(E, r) \quad (14)$$

In the region outside the sphere  $S$  the radial function  $R_{\ell}$  satisfies the differential equation

$$\frac{d^2 R_{\ell}}{dr^2} + \frac{2}{r} \frac{dR_{\ell}}{dr} + \left[ 2(E+V) - \frac{\ell(\ell+1)}{r^2} \right] R_{\ell} = 0 \quad (15)$$

with the solution :

$$R_{\ell} = A_{\ell} j_{\ell}(\gamma r) + B_{\ell} n_{\ell}(\gamma r) \quad (16)$$

This is independent of the boundary conditions ,

$$\text{where } \gamma = \sqrt{2(E+V)} \quad (17)$$

Here ,  $j_{\ell}$  and  $n_{\ell}$  are spherical Bessel functions ,  
the normal derivative of 14 - including only

$j_{\ell}$  - takes the following form :

$$\sum_{\ell t} C_{\ell t} \left[ \frac{\partial K_{\ell t}}{\partial n} j_{\ell}(\gamma r) + \gamma K_{\ell t} \cos \theta \frac{dj_{\ell}(\gamma r)}{d(\gamma r)} \right] \quad (18)$$

The explanation of  $\Theta$  is given on page 27 .

According to the tables of Bouckaert , Smoluchowski and Wigner , a wave function corresponding to  $K = \frac{\pi}{a}(0.0.0)$  must be of the basic symmetry type  $\Gamma_1$  . It is a full cubic group and we may expect one of the low energy states for the crystal . In this particular case , we may assume an expansion up to  $\ell=5$  to be an accurate enough solution. Our expansion of the wave function will then contain only two terms.

It will be convenient to use the unnormalised Cubic Harmonics

$$K_0=1 \quad \text{and} \quad K_4 = \frac{x^4 + y^4 + z^4}{r^4} - \frac{3}{5} \quad (19)$$

absorbing the normalisation into the  $C_{\ell m}$ , to find

$\frac{\partial K_n}{\partial n}$ , letting  $K_n = f$ . As to the  $xy$  plane for which the function  $f(xy)$  is defined, it has been pointed out that its normal derivative can be expressed as

$$\frac{\partial f}{\partial n} = \frac{\partial f}{\partial x} \cos \alpha_1 + \frac{\partial f}{\partial y} \cos \alpha_2 \quad (20)$$

for a plane parallel to the  $z$  axis . In our case , this relationship is simplified owing to the fact that  $\alpha_1 = \alpha_2 = \frac{1}{\sqrt{2}}$

The functions of  $J_\ell$  and  $n_\ell$  - occurring in the solution of the radial function  $R_\ell$  - have been termed spherical Bessel functions . The interesting feature of these half - order functions is that their series converge to relatively simple trigonometric functions

$$J_0(x) = \frac{\sin x}{x} \qquad n_0(x) = \frac{\cos x}{x}$$

$$J_1(x) = \frac{\sin x}{x^2} - \frac{\cos x}{x} \qquad n_1(x) = -\frac{\sin x}{x} - \frac{\cos x}{x^2}$$

The well known " derivative " recurrence formulae establish relationships between Bessel functions of various orders , and there is no reason why they should not be applied here . However ,  $J$  and  $n$  , the signs of derivative of zero order , have to be considered separately . Finally page 27 shows that  $\cos \theta = \frac{1}{\sqrt{2}}$

The coordinates of the vector tip  $\gamma'$  are ,  
in fact , equal to those of  $\gamma$  with a -ve sign  
for  $x$  and  $y$ ,  $(\gamma'(xy) \rightarrow \gamma(yx))$  This has no  
effect whatsoever on the evaluation of the integrals  
(  $x$  and  $y$  are of even powers in the case  $\gamma$  or  $\gamma'$  )  
and we may thus say that  $\gamma' = \gamma$

When we substitute 14 using 18 into 13 , the  
number of integrals to be evaluated is reduced by  
the above properties , and the similarity from 32  
to 21 . ( page28-30) .

THE ANGLE  $\theta$

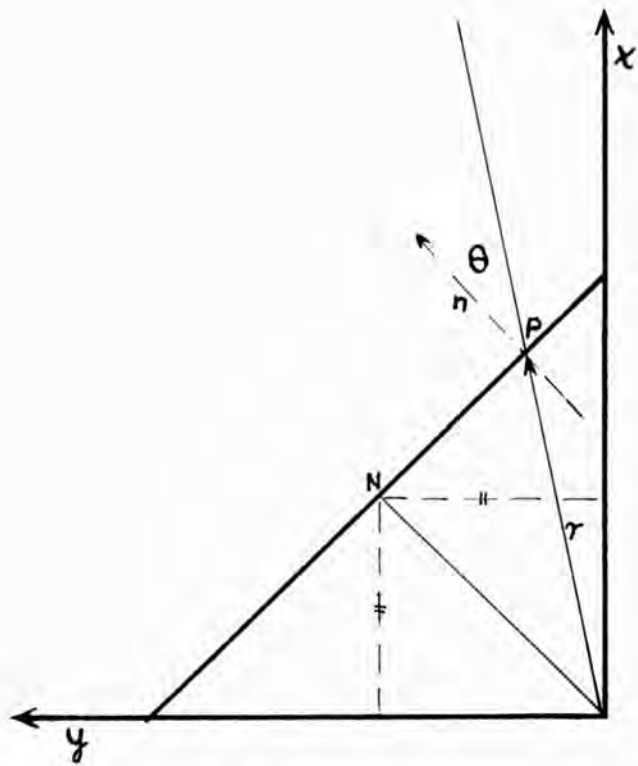


Fig. 3

$\theta$  is the angle between the vectors  $(\gamma, n)$  with the point P moving over the surface a b c d ( Fig.2 page 14 ).

TABLE OF INTEGRALS

$$1 \quad - \frac{C_0^2 A_0^2}{\sqrt{2}} \int_s X f_1(\vartheta r) f_0(\vartheta r) ds$$

$$2 \quad \frac{C_0^2 B_0^2}{\sqrt{2}} \int_s X n_1(\vartheta r) n_0(\vartheta r) ds$$

$$3 \quad \frac{C_0^2 A_0 B_0}{\sqrt{2}} \int_s X \{n_1(\vartheta r) f_0(\vartheta r) - f_1(\vartheta r) n_0(\vartheta r)\} ds$$

$$4 \quad \frac{C_0 C_4 A_0 A_4}{2\sqrt{2}} \int_s X Y \{f_3(\vartheta r) - f_5(\vartheta r)\} f_0(\vartheta r) ds$$

$$5 \quad \frac{C_0 C_4 A_4 B_0}{2\sqrt{2}} \int_s X Y \{f_3(\vartheta r) - f_5(\vartheta r)\} n_0(\vartheta r) ds$$

$$6 \quad \frac{C_0 C_4 B_0 B_4}{2\sqrt{2}} \int_s X Y \{n_5(\vartheta r) - n_3(\vartheta r)\} n_0(\vartheta r) ds$$

$$7 \quad \frac{C_0 C_4 A_0 B_4}{2\sqrt{2}} \int_s X Y \{n_5(\vartheta r) - n_3(\vartheta r)\} f_0(\vartheta r) ds$$

$$8 \quad - \frac{C_0 C_4 A_0 A_4}{\sqrt{2}} \int_s X Y f_1(\vartheta r) f_4(\vartheta r) ds$$

$$9 \quad - \frac{C_0 C_4 A_0 B_4}{\sqrt{2}} \int_s X Y f_1(\vartheta r) n_4(\vartheta r) ds$$

TABLE OF INTEGRALS

$$10 \quad \frac{C_0 C_4 B_0 B_4}{\sqrt{2}} \int_s X Y n_1(\vartheta r) n_4(\vartheta r) ds$$

$$11 \quad \frac{C_0 C_4 A_4 B_0}{\sqrt{2}} \int_s X Y n_1(\vartheta r) j_4(\vartheta r) ds$$

$$12 \quad \frac{C_4^2 A_4^2}{2\sqrt{2}} \int_s X Y^2 \{j_3(\vartheta r) - j_5(\vartheta r)\} j_4(\vartheta r) ds$$

$$13 \quad \frac{C_4^2 B_4^2}{2\sqrt{2}} \int_s X Y^2 \{n_5(\vartheta r) - n_3(\vartheta r)\} n_4(\vartheta r) ds$$

$$14 \quad \frac{C_4^2 A_4 B_4}{2\sqrt{2}} \int_s X Y^2 \left\{ [j_3(\vartheta r) - j_5(\vartheta r)] n_4(\vartheta r) + \right. \\ \left. + [n_5(\vartheta r) - n_3(\vartheta r)] j_4(\vartheta r) \right\} ds$$

$$15 \quad \frac{4C_0 C_4 A_0 A_4}{\sqrt{2}} \int_s Z j_4(\vartheta r) j_0(\vartheta r) ds$$

$$16 \quad \frac{4C_0 C_4 A_4 B_0}{\sqrt{2}} \int_s Z j_4(\vartheta r) n_0(\vartheta r) ds$$

$$17 \quad \frac{4C_0 C_4 B_0 B_4}{\sqrt{2}} \int_s Z n_4(\vartheta r) n_0(\vartheta r) ds$$



TABLE OF INTEGRALS

$$18 \quad \frac{4C_0 C_4 A_0 B_4}{\sqrt{2}} \int_s Z n_4(\partial r) f_0(\partial r) ds$$

$$19 \quad \frac{4C_4^2 A_4^2}{\sqrt{2}} \int_s Z Y \{f_4(\partial r)\}^2 ds$$

$$20 \quad \frac{4C_4^2 B_4^2}{\sqrt{2}} \int_s Z Y \{n_4(\partial r)\}^2 ds$$

$$21 \quad \frac{8C_4^2 A_4 B_4}{\sqrt{2}} \int_s Z Y \{n_4(\partial r) f_4(\partial r)\} ds$$

$$\frac{\delta}{\gamma} = X$$

$$\frac{x^4 + y^4 + z^4}{r^4} - \frac{3}{5} = Y$$

$$\frac{r^2(x^3 + y^3) - (x^4 + y^4 + z^4)(x + y)}{r^6} = Z$$

THE EMPTY LATTICE TEST

One of the methods used for testing the suitability of arbitrarily chosen boundary point conditions is the empty lattice test . This test has been devised by W. Shockley to obtain a critical evaluation of the rigour of the cellular method in deriving energy levels and wave functions in solids . It consists in applying the cellular method to the only case where an exact solution is possible , and comparing the results obtained with the optimum . This is the trial case of the empty space .

The wave function is expanded in lattice harmonics in each  $W - S$  cell , the radial functions being the well - known spherical Bessel functions whose numerical values have been obtained from the standard tables ( Tables of Spherical Bessel Functions 2 vols. Columbia Univ. Press . 1947 . )

Originally , Schockley results were used to show that, with the exception of the cases with low energy states of the crystal , an excessive number of terms is needed for the expansion of a wave function . This difficulty has been largely removed by the restriction of the calculation to the special symmetry points of B . Z .

a) The approximate method of calculation using 'W-S' assumption

We use for each cell eq. 14. The approximation of replacing the polyhedron cell by the equivalent sphere is most accurate, when the Bloch function appropriate to  $k=0$  has the full symmetry of the lattice, so that it is, in most cases, nearly  $s$ -like in the neighbourhood of an ion. In spherical approximation, the wave function is actually an  $s$  function in each cell. The approximation may also be expected to be good, when the  $k$  vector is not too close to the surface of the B. Z. Brooks has demonstrated that, under these circumstances, the sphere of equal volume is likely to yield the best energy results when the boundary conditions e.g. 2 and 3 are used, provided the wave function is in spherical approximation an  $s$  function, and with the further proviso that wave function and potential are nearly constant in the volume between the surface of the equivalent sphere and the surface of the polyhedron cell.

Let us assume, in the light of the above facts, that  $a$  is the size of the elementary cube. In this

case the volume will equal  $a^3$  ( page 36 ) . There are 4 atoms in the elementary cube , hence the volume of each cell is  $\frac{a^3}{4}$  . The radius of the equal volume sphere is  $R$

$$\frac{4\pi}{3}R^3 = \frac{a^3}{4} \quad R = a\sqrt{\frac{3}{16\pi}} = 0.391a \quad (21)$$

If we take only one term in  $\psi_k$  expansion , the boundary condition will be  $\left(\frac{\partial\psi_k}{\partial r}\right)_{r=R} = 0$  and  $j_0(\gamma r)$  , vanishing at zero value of the argument :

$$\gamma R = 4.4935$$

$$\gamma = \frac{4.4935}{0.391a} = \frac{11.49}{a} \quad E \approx \frac{66}{a^2} \quad (22)$$

in the spherical approximation.

b) The exact method of calculation  $E$

The energies obtained by the cellular method may be compared with the exact solution of the empty lattice problem. For the face centred cubic lattice, the two sets of shortest  $K$  vectors (reciprocal vector) are

$$K = \frac{\hat{r}}{a} (\pm 1, \pm 1, \pm 1) \quad \text{set of 8} \quad (23)$$

$$K = \frac{\hat{r}}{a} (\pm 2, 0, 0) \quad \text{set of 6}$$

The vectors being sufficient to specify the first zone. Hence, the first B.Z. is a truncated octahedron. The true wave functions are, in fact, plane waves - in this case with energies

$$E_k = \frac{\hbar^2 k^2}{2m} \quad V=0 \quad \gamma = \sqrt{2}E \quad (24)$$

or, since we are using the reduced zone scheme

$$E_k = \frac{\hbar^2 |k + K|^2}{2m} \quad (25)$$

for  $K=0$  and using Rydberg units we obtain

$$E_k = \frac{59.22}{a^2} \quad (26)$$

THE CONSTRUCTION OF CELLULAR POLYHEDRA

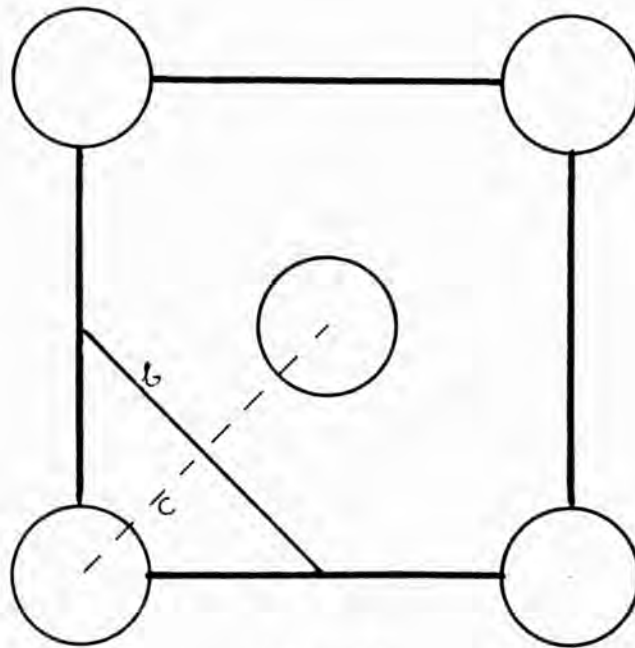


Fig. 4

The unit cell is chosen as the polyhedron of smallest volume whose plane faces (e.g. a plane b) bisect orthogonally the lines (e.g. a line c) joining the atom with its neighbours.

APPLICATION OF THE EMPTY LATTICE TEST

TO f.c.c. CRYSTAL

In the application of the empty lattice test we are faced by the problem of establishing a "free electron correspondence". The value of  $k$  completely specifies the  $\psi_k$  within each cell. The plane waves are characterised by the vectors  $K$ . The energy - bands corresponding to different values of  $K$  are degenerate in the same manner as  $l$  - type atomic levels. If a cubically symmetrical perturbation were imposed, these degenerate waves would split into different  $\Gamma$  types functions. The actual procedure illustrated here corresponds to a value of  $k=0$  for the type  $\Gamma_1$  of the wave function.

In fact, the constant potential method is very suitable for a direct application of the empty lattice test. Moreover, it can be used to judge the correct-



ness of the procedure to be employed in the calculation of the " real case " .

Here , the number of integrals to be evaluated over the quarter of the face of the polyhedron ( full cubic group ) is reduced from 21 to 6 by taking

$$n(\gamma r) = 0 \text{ ( page 32 ) .}$$

The second - kind Bessel function  $n(\gamma r)$  has singularity at  $r=0$  , and is hence discarded in the problems where  $R_e(Er)$  must remain finite or more precisely , where the coefficients of these terms  $B_e$  must be equal zero.

TABLE OF INTEGRALS ( EMPTY LATTICE TEST )

$$1 \quad - \frac{C_0^2 A_0^2}{\sqrt{2}} \int_s X f_1(\sigma r) f_0(\sigma r) ds$$

$$4 \quad \frac{C_0 C_4 A_0 A_4}{2\sqrt{2}} \int_s X Y \{ f_3(\sigma r) - f_5(\sigma r) \} f_0(\sigma r) ds$$

$$8 \quad - \frac{C_0 C_4 A_0 A_4}{\sqrt{2}} \int_s X Y f_1(\sigma r) f_4(\sigma r) ds$$

$$12 \quad \frac{C_4^2 A_4^2}{2\sqrt{2}} \int_s X Y^2 \{ f_3(\sigma r) - f_5(\sigma r) \} f_4(\sigma r) ds$$

$$15 \quad \frac{4 C_0 C_4 A_0 A_4}{\sqrt{2}} \int_s Z f_4(\sigma r) f_0(\sigma r) ds$$

$$19 \quad \frac{4 C_4^2 A_4^2}{\sqrt{2}} \int_s Z Y \{ f_4(\sigma r) \}^2 ds$$

SURFACE INTEGRAL ( NUMERICAL INTEGRATION )

To find a surface integral by the numerical method , it will be necessary first to give a brief survey of its development . This will enable us to gain a clear picture of the admissible amount of approximation which has found entry into the finally established formulae .

When we consider central differences , it is necessary to introduce two operators . These are , in Sheppards notation :

a) the central difference operator  $\delta$  defined by

$$\delta u(r) = u(r + \frac{1}{2}) - u(r - \frac{1}{2}) \quad ( 27 )$$

b) the average operator  $\mu$  is defined by

$$\mu u(r) = \frac{1}{2} \left\{ u(r + \frac{1}{2}) + u(r - \frac{1}{2}) \right\} \quad ( 28 )$$

In particular

$$\mathcal{S}U(k + \frac{1}{2}) = U_{k+1} - U_k \quad (29)$$

and

$$\mu U(k + \frac{1}{2}) = \frac{1}{2}(U_{k+1} + U_k) \quad (30)$$

the fundamental symbolic relations are

$$\mathcal{S} = E^{\frac{1}{2}} - E^{-\frac{1}{2}} \quad 2\mu = E^{\frac{1}{2}} + E^{-\frac{1}{2}} \quad (31)$$

these produce a number of useful subsidiary relations

$$E^{\frac{1}{2}} = \mu + \frac{\mathcal{S}}{2} \quad E^{-\frac{1}{2}} = \mu - \frac{\mathcal{S}}{2} \quad \mu^2 = 1 + \frac{\mathcal{S}^2}{4} \quad (32)$$

$$2\mu\mathcal{S} = E - E^{-1} \quad E = 1 + \mu\mathcal{S} + \frac{\mathcal{S}^2}{2} \quad (32)$$

To obtain Stirling's formula, we expand by the binomial theorem  $E^r$

$$E^r = \left(1 + \mu\mathcal{S} + \frac{\mathcal{S}^2}{2}\right)^r \quad \text{or} \quad \left(\mu + \frac{\mathcal{S}}{2}\right)^{2r} \quad (33)$$

$$E^r = 1 + r\mu\mathcal{S} + r_2\mathcal{S}^2 + r_3\mu\mathcal{S}^3 + r_4\mathcal{S}^4 \quad (34)$$

To obtain derivatives at tabular points , it is convenient to start with Stirling's formula . For the first few derivatives we obtain

$$\begin{aligned}
 U'(0) &= S'_0 - \frac{1}{6} S''_0 + (\frac{1}{30}) S''''_0 \text{-----} \\
 U^2(0) &= S''_0 - \frac{1}{12} S''''_0 + (\frac{1}{90}) S''''''_0 \text{-----} \\
 U^3(0) &= S'''_0 - \frac{1}{4} S''''_0 \text{-----}
 \end{aligned}
 \tag{ 35 }$$

Of the practical forms of central difference formulae Evartt's formula is superior to the others in its applicability

$$\begin{aligned}
 U(\tau) &= (1-\tau)U_0 + E_0^2 S_0^2 + E_0^4 S_0^4 \text{-----} + \\
 &+ U_1 + E_1^2 S_1^2 + E_1^4 S_1^4 \text{-----}
 \end{aligned}
 \tag{ 36 }$$

which serves as a suitable starting point and leads to the following direct derivation:

$$\psi_{rs} = \left\{ \rho + \rho_3 \Delta x^2 + \rho_5 \Delta x^4 + \dots \right\} \psi_{0s} + \left\{ \tau + \tau_3 \Delta x^2 + \tau_5 \Delta x^4 + \dots \right\} \psi_{1s} \quad (37)$$

where  $\rho = 1 - \tau$  then

$$\psi_{rs} = \left\{ \right\} \psi_{00} + \left\{ \right\} \psi_{01} + \left\{ \right\} \psi_{10} + \left\{ \right\} \psi_{11} \quad (38)$$

When suitable interpolation formulae like the ones given above have been derived, the problem of cubature, i.e. integration over a rectangular area in the  $(x, y)$  plane will prove relatively simple. There is, however, an inordinate variety of possible formulae designed to meet slightly different requirements, and only a few of these have fairly applicability. From the mid-panel formula (38) we derive

$$\int_{x_0}^{x_0 + \omega_1} dx \int_{y_0}^{y_0 + \omega_2} dy \psi(x, y) \quad (39)$$

In most cases this result is easily obtained when the interpolation formula is given in terms of differences . Its practical value is greatest , when it is expressed in Lagrangian form .

Closed Cubature formulae are often used when integrals are required over a rectangular region . There is an obvious advantage in having two formulae of comparable accuracy to apply in any particular instance , for the results are mutually checking . It is not always permissible , however , to treat the final digits , in which both answers agree, as accurate . It is evident that , in case of a discrepancy between the digits , the results are invalid and should be automatically discarded . Here we have quoted two formulae ( page 47 ) both 4 by 4 .

To estimate the value of the integral by cubature we have been forced in our case to resort to the following procedure : The parallel face to the - axis of

the rombohedron was subdivided into 4 parts . A simple transformation to the rectangular boundaries was obtained by joining one of the sectors to the edge of the rombohedron in the way pointed out on page 46 . The area was subdivided into strips of equal width , parallel to both the  $y$  and the  $x$  axis. The cross - sections of dividing lines , with their respective coordinates , were numbered and tabulated on page 48.

To calculate the integral over the quarter face,  $\frac{1}{2}$  values only were taken of the points along the edge of the rombohedron (1,9,10,14,15). The next step to take was then to add together those values which had to be multiplied by the same numerical coefficients in the cubature formula, and to find their sums. (Tables specially drawn up are on page 50-58 ). The final result was multiplied by the proper factor ( $\omega_1$  and  $\omega_2$  are intervals used in the selection of the points). In our case this was not essential, since it is only the relative value of the integrals that was required.





SURFACE INTEGRATION FORMULAE

1)

1	4	2	4	1
4	16	8	16	4
2	8	4	8	2
4	16	8	16	4
1	4	2	4	1

2)

1	6	2	6	1
6	20	12	20	6
2	12	4	12	2
6	20	12	20	6
1	6	2	6	1

a)

Factor 1/9

b)

Factor 1/12

Cubature Formulae a and b

SURFACE INTEGRATION TABLE

N	x	y	z	r <sup>2</sup>	r	Y	Y <sup>2</sup>	Z	YZ
1	1	0	0	1	1	0.40000	0.16000	0	0
2	$\frac{7}{8}$	$\frac{1}{8}$	0	25/32	0.88389	0.36080	0.13018	-0.12902	-0.04655
3	$\frac{3}{4}$	$\frac{1}{4}$	0	$\frac{5}{8}$	0.79059	0.22000	0.04840	-0.19200	-0.04224
4	$\frac{5}{8}$	$\frac{3}{8}$	0	17/32	0.72886	0.01727	0.00030	-0.09770	-0.00169
5	$\frac{1}{2}$	$\frac{1}{2}$	0	$\frac{1}{2}$	0.70711	-0.10000	0.01000	0	0
6	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{8}$	33/64	0.71809	-0.12893	0.01662	0.08014	-0.01033
7	$\frac{5}{8}$	$\frac{3}{8}$	$\frac{1}{8}$	35/64	0.73951	-0.02286	0.00052	-0.62694	0.01433
8	$\frac{3}{4}$	$\frac{1}{4}$	$\frac{1}{8}$	41/64	0.80039	0.18108	0.03279	0.91281	0.16529
9	$\frac{7}{8}$	$\frac{1}{8}$	$\frac{1}{8}$	51/64	0.89268	0.32388	0.10490	-0.10132	-0.03282
10	$\frac{3}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	11/16	0.82915	0.08595	0.00739	-0.07213	-0.00620
11	$\frac{5}{8}$	$\frac{3}{8}$	$\frac{1}{4}$	19/32	0.77055	-0.10000	0.01000	0	0
12	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{4}$	9/16	0.75000	-0.19529	0.03709	0.06584	-0.01268
13	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{3}{8}$	41/64	0.80039	-0.24723	0.06117	0.58502	-0.14469
14	$\frac{5}{8}$	$\frac{3}{8}$	$\frac{3}{8}$	43/64	0.81968	-0.17437	0.03041	0.24149	-0.04211
15	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{3}{4}$	0.86605	-0.26667	0.07111	0	0

The above table represents the coordinates x , y , z of 15 points , and the values of terms appearing in the integrals .

THE VALUE OF THE SURFACE INTEGRALS

CUBATURE FORM ' a '

In the tables 1 , 2 , 3 , 4 and 5 the first column represents the points on the surface of integration , and the last the cubature coefficients by which the remaining columns are multiplied ( top values ) . Throughout this work the integrals are referred to by the numbers assigned to them in the table on page 28,29,30.

TABLE 1.

N	$C_0^2 A_0^2$ '1'	$C_0 C_4 A_0 A_4$ '4/2'	$C_0 C_4 A_0 A_4$ '8'	$C_4^2 A_4^2$ '12/2'	$C_0 C_4 A_0 A_4$ 4×'15'	$C_4^2 A_4^2$ 4×'19'	
1/2	-0.05565	-0.00562	0.03100	0.00313			
	-0.05565	-0.00562	0.03100	0.00313			1
2	-0.28884	-0.13360	0.08772	0.04056	0.07600	-0.02304	
	-0.07221	-0.03340	0.02193	0.01014	0.01900	-0.00576	4
3	0.14712	-0.05520	-0.02206	0.00824	0.04688	-0.00704	
	0.07356	-0.02760	-0.01103	0.00414	0.02344	-0.00352	2
4	0.70916	-0.00824	-0.00812	0.00012	0.03408	-0.00032	
	0.17729	-0.00206	-0.00203	0.00003	0.00852	-0.00008	4
5	0.20192	0.01102	0.01374	0.00075			
	0.20192	0.01102	0.01374	0.00075			1
6	0.76284	0.05936	0.06584	0.00580	-0.02576	-0.00224	
	0.19071	0.01484	0.01646	0.00145	-0.00644	-0.00056	4
7	2.59248	0.04464	0.03920	0.00064	0.94724	0.01408	
	0.16203	0.00279	0.00245	0.00004	0.05880	0.00088	16
8	0.44472	-0.17976	-0.05568	0.02248	-0.92416	0.11552	
	0.05559	-0.02247	-0.00696	0.00281	-0.11552	0.01444	8
9/2	-0.65040	-0.22752	0.18240	0.06384	0.11968	-0.03392	
	-0.04065	-0.01422	0.01140	0.00399	0.00748	-0.00212	16
10/2	0.00992	-0.02008	-0.00064	0.00128	0.01984	-0.00128	
	0.00248	-0.00502	-0.00016	0.00032	0.00496	-0.00032	4
11	0.88080	0.10104	0.05872	0.00680			
	0.11010	0.01263	0.00734	0.00085			
12	0.29102	0.04788	0.03700	0.00610	-0.01816	-0.00168	
	0.14551	0.02394	0.01850	0.00305	-0.00660	-0.00084	2
13	0.22236	0.12276	0.03804	0.02100	-0.14816	-0.02528	
	0.05559	0.03069	0.00951	0.00525	-0.03704	-0.00632	4
14/2	0.16928	0.16704	0.02112	0.02080	-0.25984	-0.03328	
	0.01058	0.01044	0.00132	0.00130	-0.01624	-0.00208	16
15/2	-0.02535	0.01355	-0.00540	0.00289			
	-0.02535	0.01355	-0.00540	0.00289			1
4/1152	5.41138	-0.06673	0.48288	0.20443	-0.13384	0.00152	

$$\gamma = 5.40$$

TABLE 2

N	$C_0^2 A_0^2$ '1'	$C_0 C_4 A_0 A_4$ '4/2'	$C_0 C_4 A_0 A_4$ '8'	$C_4^2 A_4^2$ '12/2'	$C_0 C_4 A_0 A_4$ '4x15'	$C_4^2 A_4^2$ '4x19'	
1/2	-0.05206	-0.00339	0.03476	0.00226			1
2	-0.40160	-0.12032	0.13228	0.03968	0.07552	-0.02480	4
3	0.07118	-0.05650	-0.01106	0.00878	0.05056	-0.00784	2
4	0.62076	-0.00908	-0.00708	0.00012	0.03888	-0.00048	4
5	0.19018	0.01250	0.01263	0.00083			1
6	0.69404	0.06632	0.05912	0.00564	-0.02976	-0.00256	4
7	2.17344	0.04864	0.03296	0.00080	1.06304	0.01600	16
8	0.13536	-0.18192	-0.01768	0.02288	-0.98848	0.12864	8
9/2	-0.85696	-0.20176	0.26208	0.06176	0.11744	-0.03584	16
10/2	-0.06640	-0.01960	0.00876	0.00300	0.02072	-0.00136	4
11	0.60040	0.10592	0.02048	0.00364			8
12	0.23148	0.05142	0.02972	0.00662	-0.01472	-0.00184	2
13	0.06768	0.12424	0.01208	0.02212	-0.31680	-0.05632	4
14/2	-0.14080	0.16512	-0.01840	0.02160	-0.27296	-0.03584	16
15/2	-0.04159	0.01507	-0.00952	0.00288			1
	3.22511	-0.00334	0.54113	0.20261	-0.25656	-0.02224	

$$\gamma = 5.55$$



TABLE 3

N	$C_0^2 A_0^2$ '1'	$C_0 C_4 A_0 A_4$ '4/2'	$C_0 C_8 A_0 A_4$ '8'	$C_4^2 A_4^2$ '12/2'	$C_0 C_4 A_0 A_4$ '4x15'	$C_4^2 A_4^2$ '4x19'	
1/2	-0.04500	-0.00151	0.03753	0.00125			1
2	-0.48908	-0.10396	0.17704	0.03762	0.07328	-0.02656	4
3	-0.00880	-0.02599	0.00426	0.00942	0.01832	-0.00664	2
4	-0.00440	-0.02819	0.00071	0.00468	0.02672	-0.00432	4
5	0.50020	-0.00972	-0.00572	0.00012	0.04336	-0.00048	1
6	0.12505	-0.00243	-0.00143	0.00003	0.01084	-0.00012	4
7	0.16856	0.01378	0.01112	0.00091			4
8	0.16856	0.01378	0.01112	0.00091			1
9/2	0.58868	0.07204	0.05024	0.00616	-0.03360	-0.00288	4
10/2	0.14717	0.01801	0.01256	0.00154	-0.00840	-0.00072	16
11	1.63776	0.05136	0.02512	0.00080	1.17504	0.01792	8
12	0.10236	0.00321	0.00157	0.00005	0.07344	0.00112	8
13	-0.18176	-0.17928	0.02480	0.02456	1.03648	0.14176	16
14/2	-0.02272	-0.02241	0.00310	0.00307	0.12956	0.01772	8
15/2	-1.00944	-0.17104	0.34080	0.05776	0.11328	-0.03840	16
16/2	-0.06309	-0.01069	0.02130	0.00361	0.00708	-0.00240	4
17/2	-0.13860	-0.01860	0.00980	0.00128	0.02112	-0.00144	8
18/2	-0.03465	-0.00465	0.00245	0.00032	0.00528	-0.00036	4
19/2	0.28760	0.10824	0.02032	0.00768			8
20/2	0.03595	0.01353	0.00254	0.00096			2
21/2	0.15944	0.05380	0.02096	0.00708	-0.01616	-0.00208	4
22/2	0.07972	0.02690	0.01048	0.00354	-0.00808	-0.00104	4
23/2	-0.09088	0.12244	-0.01696	0.02288	-0.33216	-0.06208	16
24/2	-0.02272	0.03061	-0.00424	0.00512	-0.08304	-0.01552	4
25/2	-0.44224	0.15856	-0.06144	0.02208	-0.28160	-0.03904	16
26/2	-0.02764	0.00991	-0.00384	0.00138	-0.01760	-0.00244	1
27/2	-0.05526	0.01124	-0.01375	0.00280			1
28/2	-0.05526	0.01124	-0.01375	0.00280			1
29/1152	0.88118	0.05097	0.62128	0.20234	-0.22048	-0.02192	

$\gamma = 5.70$

TABLE 4

N	$C_0^2 A_0^2$ '1'	$C_0 C_4 A_0 A_4$ '4'/2	$C_0 C_4 A_0 A_4$ '8'	$C_4^2 A_4^2$ '12'/2	$C_0 C_4 A_0 A_4$ 4x'15'	$C_4^2 A_4^2$ 4x'19'	
1/2	-0.04382	-0.00129	0.03782	0.00111			1
2	-0.49880	-0.10164	0.18288	0.03728	0.07280	-0.02672	4
3	-0.01954	-0.05624	0.00322	0.00918	0.05376	-0.00880	2
4	0.48188	-0.00980	-0.00556	0.00012	0.04400	-0.00048	4
5	0.16470	0.01393	0.01087	0.00092			1
6	0.57224	0.07276	0.04888	0.00624	-0.03408	-0.00288	4
7	1.55936	0.05184	0.02416	0.00080	1.18912	0.01856	16
8	-0.2352	-0.17856	0.03088	0.02464	-1.04128	0.14336	8
9/2	-0.02794	-0.02232	0.00386	0.00308	-0.13016	0.01792	16
10/2	-1.02528	-0.16656	0.35120	0.05712	0.11264	-0.03840	4
11	-0.06408	-0.01041	0.02195	0.00357	0.00704	-0.00240	8
12	-0.14792	-0.01844	0.01052	0.00132	0.02128	-0.00160	2
13	-0.03698	-0.00461	0.00263	0.00033	0.00532	-0.00040	8
14/2	0.24408	0.10832	0.01736	0.00768			2
15/2	0.03051	0.01354	0.00217	0.00096	-0.01632	-0.00216	4
4/1152	0.14918	0.05402	0.01968	0.00714	-0.00816	-0.00108	4
	0.07459	0.02701	0.00984	0.00357	-0.33376	-0.06272	16
	-0.11176	0.12192	-0.02108	0.02296	-0.08344	-0.01568	16
	-0.02794	0.03048	-0.00527	0.00574	-0.28224	-0.03968	1
	-0.48128	0.15744	-0.06736	0.02208	-0.01764	-0.00248	
	-0.03008	0.00984	-0.00421	0.00138			
	-0.05687	0.01104	-0.01431	0.00278			
	-0.05687	0.01104	-0.01431	0.00278			
	0.56265	0.05874	0.62916	0.20137	-0.21408	-0.02152	

$$\gamma = 5.72$$



TABLE 5

N	$C_0^2 A_0^2$ '1'	$C_0 C_4 A_0 A_4$ '4/2'	$C_0 C_4 A_0 A_4$ '8'	$C_4^2 A_4^2$ '12/2'	$C_0 C_4 A_0 A_4$ '4 x 15'	$C_4^2 A_4^2$ '4 x 19'	
1/2	-0.03869	-0.00052	0.03875	0.00105			1
2	-0.53124	-0.09184	0.20608	0.03564	0.07072	-0.02752	4
3	-0.06206	-0.05548	0.01042	0.00932	0.05488	-0.00920	2
4	0.40488	-0.02008	-0.00472	0.00012	0.04624	-0.00048	4
5	0.14945	0.01449	0.00990	0.00096			1
6	0.48592	0.08448	0.04184	0.00648	-0.03600	-0.00304	4
7	1.23232	0.05280	0.01936	0.00080	1.24160	0.01920	16
8	-0.38840	-0.17488	0.05520	0.02488	-1.05792	0.15040	8
9/2	-1.07648	-0.14880	0.39136	0.05408	0.10880	-0.03968	16
10/2	-0.18272	-0.01764	0.01352	0.00132	0.02128	-0.00160	4
11	0.06928	0.11072	0.00504	0.00792			8
12	0.10672	0.05472	0.01432	0.00734	-0.00848	-0.00120	2
13	-0.19420	0.11944	-0.03772	0.02320	-0.33904	-0.06656	4
14/2	-0.63072	0.15200	-0.09152	0.02208	-0.28416	-0.04160	16
15/2	-0.06259	0.01020	-0.01656	0.00270			1
4/1152	-0.71853	0.08961	0.65527	0.19789	-0.18208	-0.02048	

$$\gamma = 5.80$$

THE VALUE OF SURFACE INTEGRAL  
IN CUBATURE FORM "b"

The tabulation of readings 1a 2a 3a is  
the same as cubature " a ".

TABLE 1a.

N	$C_0^2 A_0^2$ '1'	$C_0 C_4 A_0 A_4$ '4/2'	$C_0 C_4 A_0 A_4$ '8'	$C_4^2 A_4^2$ '12/2'	$C_0 C_4 A_0 A_4$ '4 x 15'	$C_4^2 A_4^2$ '4 x 19'	
1/2	-0.05206	-0.00339	0.03476	0.00226			
	-0.05206	-0.00339	0.03476	0.00226			1
2	-0.60240	-0.18048	0.19842	0.05952	0.11328	-0.03720	
	-0.10040	-0.03008	0.03307	0.00992	0.01888	-0.00620	6
3	0.07118	-0.05650	-0.01106	0.00878	0.05056	-0.00584	
	0.03559	-0.02825	-0.00553	0.00439	0.02528	-0.00392	2
4	0.93114	-0.01362	-0.01062	0.00018	0.05832	-0.00072	
	0.15519	-0.00227	-0.00177	0.00003	0.00972	-0.00012	6
5	0.19018	0.01250	0.01263	0.00083			
	0.19018	0.01250	0.01263	0.00083			1
6	1.04106	0.09948	0.08868	0.00846	-0.04464	-0.00384	
	0.17351	0.01658	0.01478	0.00141	-0.00744	-0.00064	6
7	2.71680	0.06080	0.04120	0.00100	1.32880	0.02000	
	0.13584	0.00304	0.00206	0.00005	0.06644	0.00100	20
8	0.20304	-0.27288	-0.02652	0.03432	-1.48272	0.19296	
	0.01692	-0.02274	-0.00221	0.00286	-0.12356	0.01608	12
9/2	-1.07120	-0.25220	0.32760	0.07720	0.14680	-0.04480	
	-0.05356	-0.01261	0.01638	0.00386	0.00734	-0.00224	20
10/2	-0.06640	-0.01960	0.00876	0.00300	0.02072	-0.00136	
	-0.01660	-0.00490	0.00219	0.00075	0.00518	-0.00034	4
11	0.90060	0.15888	0.06144	0.01092			
	0.07505	0.01324	0.00512	0.00091			12
12	0.23148	0.05142	0.02972	0.00662	-0.01472	-0.00184	
	0.11574	0.02571	0.01486	0.00331	-0.00736	-0.00092	2
13	0.10152	0.18636	0.01812	0.03318	-0.47520	-0.08448	
	0.01692	0.03106	0.00302	0.00553	-0.07920	-0.01408	6
14/2	-0.17600	0.02064	-0.00230	0.00270	-0.03412	-0.00448	
	-0.00880	0.01032	-0.00115	0.00135	-0.01706	-0.00224	20
15/2	-0.04159	0.01507	-0.00952	0.00288			
	-0.04159	0.01507	-0.00952	0.00288			1
	4.37735	-0.19352	0.76131	0.25185	-0.33292	0.02640	

$$\gamma = 5.55$$

TABLE 2a.

N	$C_0^2 A_0^2$ '1'	$C_0 C_4 A_0 A_4$ '4/2'	$C_0 C_4 A_0 A_4$ '8'	$C_4^2 A_4^2$ '12/2'	$C_0 C_4 A_0 A_4$ '4x15'	$C_4^2 A_4^2$ '4x19'	
1/2	-0.04500	-0.00151	0.03753	0.00125			1
2	-0.73362	-0.15594	0.26556	0.05652	0.10992	-0.03984	6
3	-0.00880	-0.05638	0.00142	0.00936	0.05344	-0.00864	2
4	0.75030	-0.01458	-0.00858	0.00018	0.06504	-0.00072	6
5	0.16856	0.01378	0.01112	0.00091			1
6	0.88302	0.10806	0.07536	0.00924	-0.05040	-0.00432	6
7	2.04720	0.06420	0.03140	0.00100	1.46880	0.00224	20
8	-0.27264	-0.26892	0.03720	0.03684	-1.55472	0.21264	12
9/2	-1.26180	-0.21380	0.42600	0.07220	0.14160	-0.04800	20
10/2	-0.13860	-0.01860	0.00980	0.00128	0.02112	-0.00144	4
11	0.43140	0.16236	0.03048	0.01152			12
12	0.07972	0.02690	0.01048	0.00354	-0.00808	-0.00104	2
13	-0.13632	0.18366	-0.02544	0.03432	-0.49824	-0.09312	6
14/2	-0.55280	0.19820	-0.07680	0.02760	-0.35200	-0.04880	20
15/2	-0.05526	0.01124	-0.01375	0.00280			1
	1.23508	0.06557	0.82226	0.27210	-0.61160	-0.03208	

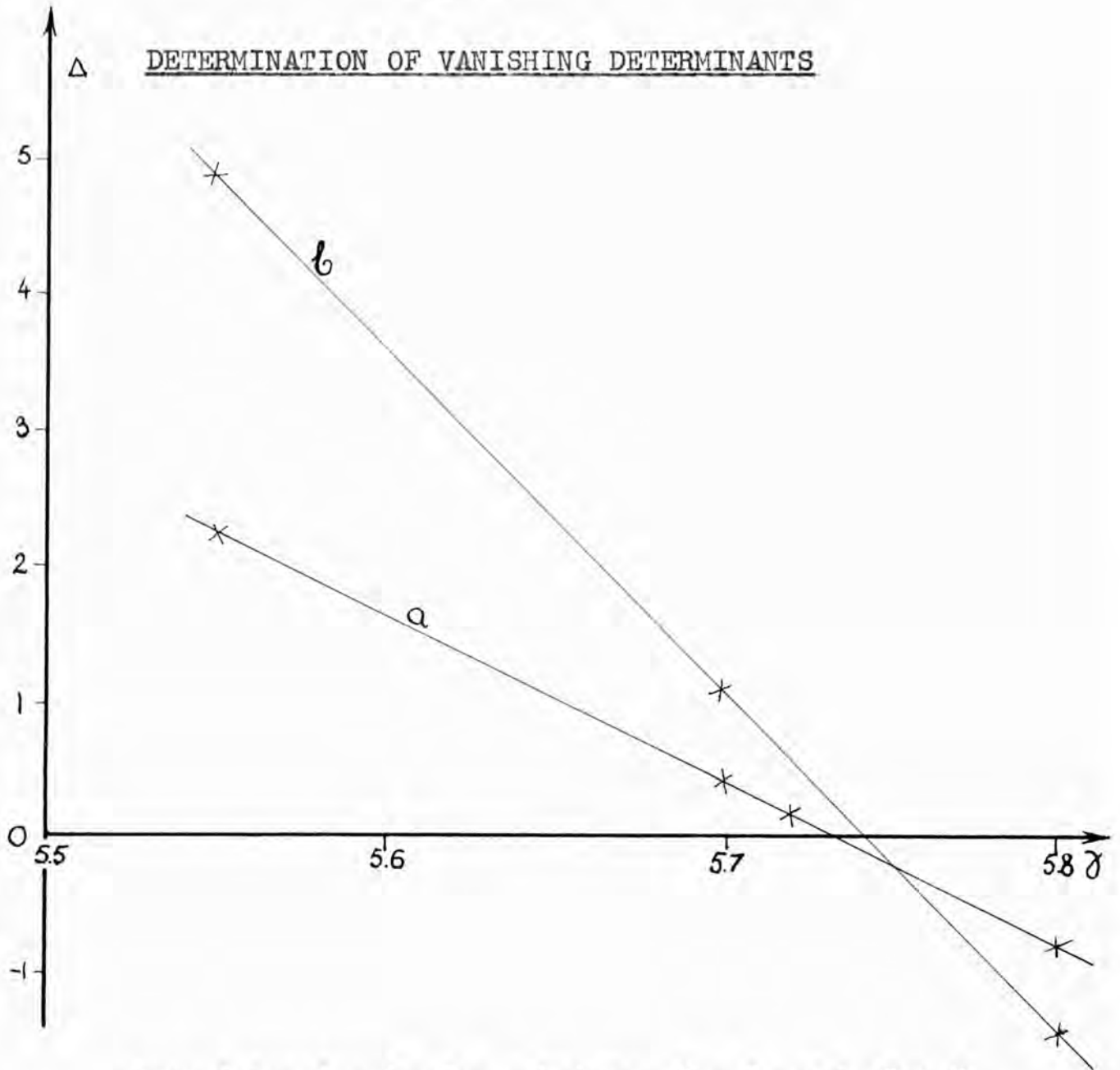
$$\gamma = 5.70$$



TABLE 3a.

N	$C_0^2 A_0^2$ '1'	$C_0 C_4 A_4$ '4/2'	$C_0 C_4 A_0 A_4$ '8'	$C_4^2 A_4^2$ '12/2'	$C_0 C_4 A_0 A_4$ '4x15'	$C_4^2 A_4^2$ '4x19'	
1/2	-0.03869	-0.00052	0.03875	0.00105			1
2	-0.79686	-0.13776	0.30912	0.05346	0.10608	-0.04128	6
3	-0.06206	-0.05548	0.01042	0.00932	0.05488	-0.00920	2
4	0.60732	-0.03012	-0.00708	0.00018	0.06936	-0.00072	6
5	0.14945	0.01449	0.00990	0.00096			1
6	0.72888	0.12672	0.06276	0.00972	-0.05400	-0.00456	6
7	1.54040	0.06600	0.02420	0.00100	1.55200	0.02400	20
8	-0.58260	-0.26232	0.08280	0.03732	-1.58688	0.22560	12
9/2	-1.34560	-0.18600	0.48920	0.06760	0.13600	-0.04960	20
10/2	-0.18272	-0.01764	0.01352	0.00132	0.02128	-0.00160	4
11	0.10392	0.16608	0.00756	0.01188			12
12	0.10672	0.05472	0.01432	0.00734	-0.00848	-0.00120	2
13	-0.29130	0.17916	-0.05658	0.03480	-0.50856	-0.09984	6
14/2	-0.78840	0.01900	-0.01144	0.00276	-0.03552	-0.00520	20
15/2	-0.06259	0.01020	-0.01656	0.00270			1
	-0.91413	-0.05347	0.97089	0.24141	-0.25384	0.03640	

$$\gamma = 5.80$$



The determinants for cubature " a " and " b " are plotted against corresponding values of  $\gamma$  .

THE METHOD OF CALCULATION

This seems the opportune moment to stress that the speed and correctness of the calculation depend , to some not unconsiderable degrees on the proper tabulation of the intermediate results .

The procedure observed here is as follows . First , the identical terms recurring in 21 integrals were tabulated ( they are mostly the products of Bessel functions and surface harmonics multiplied by  $\frac{1}{r}$  ( from  $\cos \theta$  term ), page 63-69 ) and evaluated for a number of different values of  $\gamma$  at each point . These results were then used , in turn , for the evaluation of integrals .

The most tedious task was the interpolation of the Bessel functions at different orders for each value

of  $\gamma r$ . For interpolation purposes the fourth difference is expendable over the greater portion of the main table ( Tables of Spherical Bessel Functions , N.York , Columbia Univ. Press.). Everett's formula , involving the fourth difference to

$$u(x_0 + ph) = qu_0 + pu_1 - E_2 \delta^2(u_1) - F_2 \delta^2(u_0) \quad (40)$$

$$q = 1 - p \quad u_1 = u(x_0 + h) \quad u_0 = u(x_0) \quad (41)$$

$$E_2 = E_2(p) = \frac{1}{6} p(1 - p^2) \quad F_2 = F_2(p) = E(q) \quad (42)$$

the values of  $E_2$  and  $F_2$  are tabulated against  $p$  at the end of the tables.



THE INTERPOLATED VALUES OF BESSEL FUNCTIONS  
AND THE INTERMEDIATE RESULTS  
IN THE CALCULATION OF INTEGRALS

TABLE 5

N	$\alpha$	$\gamma$	$\chi(\frac{\alpha}{\gamma})$	$f_0(\gamma r)$	$f_1(\gamma r)$	$f_2(\gamma r)$	$f_3(\gamma r)$	$f_4(\gamma r)$	$f_5(\gamma r)$	$f_6(\gamma r)$	$f_7 - f_5$
1	5.40	5.40	5.40	-0.14311	-0.14404	0.19935	0.12980	0.20245	0.07265		
	5.55	5.55	5.55	-0.12058	-0.15561	0.20123	0.13786	0.18847	0.05061		
	5.70	5.70	5.70	-0.09661	-0.16339	0.20148	0.14542	0.17270	0.02728		
	5.72	5.72	5.72	-0.09334	-0.16414	0.20138	0.14638	0.17048	0.02410		
	5.80	5.80	5.80	-0.08010	-0.16649	0.20069	0.15011	0.16131	0.01120		
2	5.40	4.77301	6.10936	-0.20913	-0.05651	0.17598	0.09347	0.23837	0.14490		
	5.55	4.90059	6.27906	-0.20005	-0.07991	0.18274	0.10125	0.23402	0.13277		
	5.70	5.03817	6.44877	-0.18804	-0.10085	0.18862	0.10905	0.22783	0.11878		
	5.72	5.05585	6.47139	-0.18624	-0.10344	0.18932	0.11010	0.22692	0.11682		
	5.80	5.12656	6.56190	-0.17857	-0.11333	0.19198	0.11423	0.22281	0.10858		
3	5.40	4.26319	6.83034	-0.21160	0.05088	0.14422	0.06522	0.23882	0.17360		
	5.55	4.38778	7.02007	-0.21600	0.02346	0.15237	0.07158	0.24096	0.16938		
	5.70	4.50636	7.20981	-0.21721	-0.00280	0.16016	0.07813	0.24174	0.16361		
	5.72	4.52218	7.23510	-0.21715	-0.00621	0.16117	0.07903	0.24174	0.16271		
	5.80	4.58542	7.33629	-0.21633	-0.01956	0.16512	0.08261	0.24149	0.15888		
4	5.40	3.93584	7.40883	-0.18125	0.13201	0.12019	0.04878	0.22607	0.17729		
	5.55	4.04517	7.61463	-0.19419	0.10496	0.12819	0.05392	0.23128	0.17736		
	5.70	4.15450	7.82043	-0.20420	0.07828	0.13610	0.05932	0.23552	0.17620		
	5.72	4.16908	7.84787	-0.20532	0.07475	0.13715	0.06005	0.23600	0.17595		
	5.80	4.22739	7.95763	-0.20927	0.06077	0.14129	0.06304	0.23776	0.17472		
5	5.40	3.81839	7.63672	-0.16402	0.16121	0.11158	0.04355	0.21943	0.17588		
	5.55	3.92446	7.84885	-0.17972	0.13484	0.11935	0.04827	0.22547	0.17720		
	5.70	4.03053	8.06098	-0.19262	0.10857	0.12712	0.05322	0.23065	0.17743		
	5.72	4.04467	8.08927	-0.19415	0.10489	0.12815	0.05390	0.23127	0.17737		
	5.80	4.10124	8.20240	-0.19969	0.09122	0.13226	0.05666	0.23359	0.17693		

TABLE 5

N	$\alpha$	$\gamma$	$\chi(\frac{\alpha}{\gamma})$	$f_0(\gamma)$	$f_1(\gamma)$	$f_4(\gamma)$	$f_5(\gamma)$	$f_3(\gamma)$	$f_3 - f_5$
6	5.40	3.87769	7.51995	-0.17314	0.14647	0.11592	0.04615	0.22290	0.17675
	5.55	3.98540	7.72884	-0.18748	0.11972	0.12383	0.05108	0.22855	0.17747
	5.70	4.09311	7.93772	-0.19894	0.09320	0.13168	0.05625	0.23326	0.17691
	5.72	4.10748	7.96558	-0.20025	0.08969	0.13271	0.05696	0.23382	0.17686
	5.80	4.16492	8.07698	-0.20500	0.07334	0.13685	0.05984	0.23587	0.17603
7	5.40	3.99335	7.30213	-0.18842	0.11776	0.12441	0.05145	0.22893	0.17748
	5.55	4.10428	7.50497	-0.20000	0.09048	0.13248	0.05681	0.23371	0.17690
	5.70	4.21521	7.70781	-0.20852	0.06368	0.14043	0.06242	0.23741	0.17499
	5.72	4.2300	7.73485	-0.20943	0.06016	0.14147	0.06318	0.23783	0.17465
	5.80	4.28916	7.84303	-0.21257	0.04620	0.14567	0.06628	0.23927	0.17299
8	5.40	4.32211	6.74671	-0.21397	0.03852	0.14789	0.06803	0.23994	0.17191
	5.55	4.44217	6.93412	-0.21695	0.01126	0.15599	0.07456	0.24150	0.16694
	5.70	4.56222	7.12153	-0.21673	-0.01471	0.16370	0.08129	0.24163	0.16034
	5.72	4.57823	7.14652	-0.21646	-0.01807	0.16468	0.08220	0.24154	0.15934
	5.80	4.64226	7.24647	-0.21488	-0.03119	0.16857	0.08587	0.24093	0.15506
9	5.40	4.82047	6.04920	-0.20624	-0.06516	0.17849	0.09625	0.23702	0.14077
	5.55	4.95437	6.21723	-0.19596	-0.08792	0.18501	0.10413	0.23195	0.12782
	5.70	5.08828	6.38527	-0.18281	-0.10808	0.19058	0.11193	0.22510	0.11311
	5.72	5.10613	6.40767	-0.18085	-0.11056	0.19125	0.11304	0.22405	0.11101
	5.80	5.17754	6.49729	-0.17263	-0.11998	0.19372	0.11719	0.21954	0.10235
10	5.40	4.47741	6.51269	-0.21720	0.00348	0.15831	0.07652	0.24168	0.16516
	5.55	4.60178	6.69360	-0.21598	-0.02295	0.16613	0.08355	0.24136	0.15781
	5.70	4.72616	6.87451	-0.21156	-0.04766	0.17341	0.09073	0.23948	0.14875
	5.72	4.74274	6.89863	-0.21075	-0.05084	0.17434	0.09170	0.23912	0.14742
	5.80	4.80907	6.99512	-0.20697	-0.06312	0.17790	0.09558	0.23737	0.14179

TABLE 5

N	$\alpha$	$\gamma\alpha$	$\chi(\frac{\alpha}{\gamma})$	$f_0(\gamma\alpha)$	$f_1(\gamma\alpha)$	$f_4(\gamma\alpha)$	$f_5(\gamma\alpha)$	$f_3(\gamma\alpha)$	$f_3 - f_5$
11	5.40	4.16097	7.00798	-0.20470	0.07672	0.13656	0.05964	0.23574	0.17610
	5.55	4.27655	7.20265	-0.21197	0.04915	0.14474	0.06561	0.23899	0.17338
	5.70	4.39214	7.39731	-0.21610	0.02248	0.15266	0.07182	0.24102	0.16920
	5.72	4.40755	7.42327	-0.21643	0.01899	0.15369	0.07266	0.24118	0.16852
	5.80	4.46919	7.52709	-0.21717	0.00529	0.15777	0.07606	0.24165	0.16559
12	5.40	4.05000	7.20000	-0.19470	0.10378	0.12854	0.05416	0.23149	0.17733
	5.55	4.16250	7.40000	-0.20482	0.07634	0.13667	0.05971	0.23579	0.17608
	5.70	4.27500	7.60000	-0.21190	0.04952	0.14463	0.06554	0.23896	0.17342
	5.72	4.29000	7.62667	-0.21261	0.04600	0.14568	0.06632	0.23929	0.17297
	5.80	4.35000	7.73333	-0.21436	0.03208	0.14981	0.06953	0.24042	0.17089
13	5.40	4.32211	6.74671	-0.21397	0.03852	0.14789	0.06803	0.23994	0.17191
	5.55	4.44217	6.93421	-0.21695	0.01126	0.15599	0.07456	0.24150	0.16694
	5.70	4.56222	7.12153	-0.21673	-0.01471	0.16370	0.08129	0.24163	0.16034
	5.72	4.57823	7.14652	-0.21646	-0.01807	0.16468	0.08220	0.24154	0.15934
	5.80	4.64226	7.24647	-0.21488	-0.03119	0.16857	0.08587	0.24092	0.15506
14	5.40	4.42627	6.58794	-0.21674	0.01479	0.15494	0.07369	0.24137	0.16768
	5.55	4.54922	6.77094	-0.21690	-0.01197	0.16288	0.08054	0.24168	0.16114
	5.70	4.67218	6.95393	-0.21386	-0.03717	0.17032	0.08760	0.24049	0.15289
	5.72	4.68857	6.97833	-0.21323	-0.04040	0.17127	0.08855	0.24021	0.15166
	5.80	4.75414	7.07593	-0.21016	-0.05299	0.17496	0.09236	0.23886	0.14650
15	5.40	4.67667	6.23521	-0.21369	-0.03805	0.17058	0.08786	0.24043	0.15257
	5.55	4.80658	6.40841	-0.20713	-0.06266	0.17777	0.09543	0.23744	0.14201
	5.70	4.93649	6.58161	-0.19751	-0.08502	0.18419	0.10307	0.23274	0.12967
	5.72	4.95381	6.60470	-0.19601	-0.08783	0.18498	0.10410	0.23198	0.12788
	5.80	5.02309	6.69707	-0.18955	-0.09861	0.18799	0.10817	0.22867	0.12050

VALUES OF INTEGRALS

The first vertical column represents 15 points on the surface of integration, and the first horizontal the particular integrals used.



TABLE 6.

N	1	4	8	12	15	19
1	-0.11129	-0.02246	0.06199	0.01251		
	-0.10412	-0.01354	0.06951	0.00904		
	-0.09000	-0.00602	0.07506	0.00501		
	-0.08763	-0.00515	0.07564	0.00444		
	-0.07737	-0.00208	0.07749	0.00209		
2	-0.07221	-0.06673	0.02193	0.02029	0.00475	-0.00144
	-0.10040	-0.06017	0.03307	0.01983	0.00472	-0.00155
	-0.12227	-0.05198	0.04426	0.01881	0.00458	-0.00166
	-0.12470	-0.05081	0.04572	0.01863	0.00455	-0.00167
	-0.13281	-0.04591	0.05152	0.01782	0.00442	-0.00172
3	0.07356	-0.05519	-0.01103	0.00828	0.00586	-0.00088
	0.03559	-0.05650	-0.00553	0.00877	0.00632	-0.00098
	-0.00440	-0.05637	0.00071	0.00914	0.00668	-0.00108
	-0.00977	-0.05624	0.00161	0.00918	0.00672	-0.00110
	-0.03103	-0.05547	0.00521	0.00931	0.00686	-0.00115
4	0.17729	-0.00411	-0.00203	0.00005	0.00213	-0.00002
	0.15519	-0.00453	-0.00177	0.00005	0.00243	-0.00003
	0.12505	-0.00486	-0.00143	0.00006	0.00211	-0.00003
	0.12047	-0.00490	-0.00139	0.00006	0.00275	-0.00003
	0.10122	-0.00502	-0.00118	0.00006	0.00289	-0.00003
5	0.20192	0.02203	0.01374	0.00150		
	0.19018	0.02500	0.01263	0.00166		
	0.16856	0.02755	0.01112	0.00182		
	0.16470	0.02786	0.01087	0.00184		
	0.14945	0.02898	0.00990	0.00192		
6	0.19071	0.02967	0.01646	0.00290	-0.00161	-0.00014
	0.17351	0.03315	0.01478	0.00282	-0.00186	-0.00016
	0.14717	0.03602	0.01256	0.00307	-0.00210	-0.00018
	0.14306	0.03638	0.01222	0.00311	-0.00213	-0.00018
	0.12148	0.04224	0.01046	0.00323	-0.00225	-0.00019

TABLE 6.

N	1	4	8	12	15	19
7	0.16203	0.00558	0.00245	0.00008	0.01470	0.00022
	0.13584	0.00607	0.00206	0.00009	0.01661	0.00025
	0.10236	0.00642	0.00157	0.00010	0.01836	0.00028
	0.09746	0.00647	0.00151	0.00010	0.01858	0.00029
	0.07702	0.00659	0.00121	0.00010	0.01940	0.00030
8	0.05559	-0.04493	-0.00696	0.00562	-0.02888	0.00361
	0.01692	-0.04548	-0.00221	0.00592	-0.03089	0.00402
	-0.02272	-0.04481	0.00310	0.00613	-0.03239	0.00443
	-0.02794	-0.04463	0.00386	0.00615	-0.03254	0.00448
	-0.04855	-0.04372	0.00690	0.00621	-0.03306	0.00470
9	-0.08130	-0.05688	0.02279	0.01595	0.00373	-0.00105
	-0.10712	-0.05044	0.03276	0.01542	0.00367	-0.00112
	-0.12617	-0.04277	0.04260	0.01444	0.00353	-0.00119
	-0.12815	-0.04165	0.04389	0.01427	0.00351	-0.00120
	-0.13456	-0.03719	0.04891	0.01352	0.00339	-0.00123
10	0.00495	-0.02008	-0.00031	0.00126	0.00248	-0.00015
	-0.03320	-0.01961	0.00219	0.00130	0.00250	-0.00017
	-0.06930	-0.01859	0.00489	0.00131	0.00264	-0.00018
	-0.07395	-0.01842	0.00525	0.00131	0.00265	-0.00019
	-0.09136	-0.01765	0.00675	0.00135	0.00266	-0.00019
11	0.11010	0.02526	0.00734	0.00169		
	0.07505	0.02647	0.00512	0.00181		
	0.03595	0.02705	0.00254	0.00191		
	0.03051	0.02707	0.00217	0.00192		
	0.00866	0.02767	0.00063	0.00197		
12	0.14551	0.04788	0.01850	0.00609	-0.00165	-0.00021
	0.11574	0.05141	0.01486	0.00661	-0.00184	-0.00023
	0.07972	0.05379	0.01048	0.00707	-0.00202	-0.00026
	0.07459	0.05402	0.00984	0.00713	-0.00204	-0.00027
	0.05336	0.05472	0.00716	0.00734	-0.00212	-0.00029

TABLE 6.

N	1	4	8	12	15	19
13	0.05559	0.06137	0.00951	0.01049	-0.01851	-0.00316
	0.01692	0.06212	0.00302	0.01105	-0.01980	-0.00352
	-0.02272	0.06121	-0.00424	0.01144	-0.02076	-0.00388
	-0.02794	0.06096	-0.00527	0.01147	-0.02086	-0.00392
	-0.04855	0.05972	-0.00943	0.01159	-0.02119	-0.00411
14	0.02115	0.04175	0.00263	0.00521	-0.00811	-0.00101
	-0.01760	0.04126	-0.00230	0.00541	-0.00853	-0.00112
	-0.05528	0.03965	-0.00768	0.00551	-0.00880	-0.00122
	-0.06015	0.03935	-0.00842	0.00551	-0.00882	-0.00124
	-0.07883	0.03799	-0.01144	0.00552	-0.00888	-0.00129
15	-0.05069	0.05421	-0.01079	0.01154		
	-0.08318	0.05028	-0.01904	0.01151		
	-0.11051	0.04495	-0.02749	0.01118		
	-0.11373	0.04416	-0.02862	0.01111		
	-0.12517	0.04079	-0.03311	0.01079		



### RESULTS

Since , in our case , the trial functions satisfy the wave equation , the relevant variational principle is eq. 12 . If we now perform the variation by varying the coefficients  $C_{lt}$  of the terms in the lattice-harmonic expression , we obtain a set of linear equations which lead to a compatibility equation of the type

$$\frac{\partial I_2}{\partial C_0} = \frac{\partial I_2}{\partial C_4} = 0 \quad ( 43 )$$

as shown on page 71-73. The equations are compatible only, if the determinant of the coefficients of  $C_{lt}$  vanishes . This will occur only with certain discrete energies  $E_K$  ( or  $\gamma$  ) .

For the empty lattice test the following determinants corresponding to : 5.4 , 5.7 , 5.72 and 5.8 have been calculated ( page 59 and 71-73). A determinant vanishes at  $\gamma = 5.73$

$$E_K = \frac{65.67}{a^2}$$

LINEAR EQUATIONS ( FOR CUBATURE ' a ' )

$$\gamma = 5.40$$

$$I_2 = 5.41138 A_0^2 C_0^2 + 0.28631 A_0 A_4 C_0 C_4 + 0.20595 A_4^2 C_4^2$$

$$\Delta = \begin{array}{cc} 10.82276 & 0.28631 \\ 0.28631 & 0.41190 \end{array} = 4.37593$$

$$\gamma = 5.55$$

$$I_2 = 3.22511 A_0^2 C_0^2 + 0.28123 A_0 A_4 C_0 C_4 + 0.18037 A_4^2 C_4^2$$

$$\Delta = \begin{array}{cc} 6.45022 & 0.28123 \\ 0.28123 & 0.36074 \end{array} = 2.24776$$

$$\gamma = 5.70$$

$$I_2 = 0.88118 A_0^2 C_0^2 + 0.45177 A_0 A_4 C_0 C_4 + 0.18042 A_4^2 C_4^2$$

$$\Delta = \begin{array}{cc} 1.76236 & 0.45177 \\ 0.45177 & 0.36084 \end{array} = 0.43183$$

LINEAR EQUATIONS ( FOR CUBATURE ' a ' )

$$\gamma = 5.72$$

$$I_2 = 0.56265 A_0^2 C_0^2 + 0.47382 A_0 A_4 C_0 C_4 + 0.17985 C_0 C_4$$

$$\Delta = \begin{array}{cc} 1.12530 & 0.47382 \\ 0.47382 & 0.35970 \end{array} = 0.18026$$

$$\gamma = 5.80$$

$$I_2 = -0.71853 A_0^2 C_0^2 + 0.56280 A_0 A_4 C_0 C_4 + 0.17741 A_4^2 C_4^2$$

$$\Delta = \begin{array}{cc} -1.43706 & 0.56280 \\ 0.56280 & 0.35482 \end{array} = -0.82664$$

$\gamma$	$\Delta$
5.40	4.37593
5.55	2.24776
5.70	0.43183
5.72	0.18026
5.80	-0.82664

LINEAR EQUATIONS ( FOR CUBATURE ' b ' )

$$\gamma = 5.55$$

$$I_2 = 4.37735 A_0^2 C_0^2 + 0.23487 A_0 A_4 C_0 C_4 + 0.27825 A_4^2 C_4^2$$

$$\Delta = \begin{array}{ccc} 8.75470 & 0.23487 & \\ & & = 4.82559 \\ 0.23487 & 0.55750 & \end{array}$$

$$\gamma = 5.70$$

$$I_2 = 1.23508 A_0^2 C_0^2 + 0.27623 A_0 A_4 C_0 C_4 + 0.24002 A_4^2 C_4^2$$

$$\Delta = \begin{array}{ccc} 2.47016 & 0.27623 & \\ & & = 1.10948 \\ 0.27623 & 0.48004 & \end{array}$$

$$\gamma = 5.80$$

$$I_2 = -0.91413 A_0^2 C_0^2 + 0.66358 A_0 A_4 C_0 C_4 + 0.27781 A_4^2 C_4^2$$

$$\Delta = \begin{array}{ccc} -1.82826 & 0.66358 & \\ & & = -1.45616 \\ 0.66358 & 0.55562 & \end{array}$$

$\gamma$	$\Delta$
5.55	4.82559
5.70	1.10948
5.80	-1.45616

$\Gamma$  AND  $E(k)$  FOR Al

In the case of  $k=0$  , the full s-band for Al is of the type  $\Gamma_1$  , containing spherical harmonics of the order 0. 4. 6. 8. ....In his paper ( Proc. of the Royal Soc. A. vol. 240 p.340 - 735 1957 ) Heine finds that the energy , corresponding to the above condition , amounts to  $-0.637 R_y$  . This proves that the argument of the Bessel function must be imaginary. Since the search for the appropriate tables was unsuccessful , and the attempt to calculate Bessel functions up to order 5 of both kinds proved too laborious a task and has had to be abandoned , the only way out of the predicament was to establish tables up to order 1 ( Tables with interval 0.01 from 0-100 , Appendix I ). Thus , instead of being evaluated from the determinants of the coefficients of  $C_{lt}$  , energy had to be determined from the surface integral .

CONSTANT POTENTIAL CALCULATION

The task here was to find the " constant potential "  $V_c$  . The method employed was as follows : the space between the inscribed and the circumscribed spheres of the polyhedron was filled with equipotential spheres , separated by a constant interval . These equipotential spheres are , in our case , of three different types . Whether a type can exist in certain regions depends on the length of the radius . The first type, with a circular base which must be subtracted from the sphere , is located in the region between 0.70711 - 0.74162 ( page 78 and 81 ). Outside this space we are left with the pyramids cut off from the polyhedron by the equipotential spheres . There are two types , both shown on page 79-80. For the sake of convenience, the spherically shaped bases of the pyramids are taken here to be flat planes . This is an approximation which refers merely to the conditions stated last , and is necessary to avoid long and tedious calculations which could hardly do more than influence the final result in the last two figures .

The region of triangular and square planes extends to 0.86605 . The last part left is filled with squares only. The formulae used for each type ( in calculation of  $A_r$  ) are quoted at the side of the figure they refer to ( page 79 and 80 ) .

The constant potential is subsequently evaluated by using the relation

$$V_c = \frac{\sum_n A_r V_r}{\sum_n A_r} \quad ( 44 )$$

( tables on page 81 ) where  $A_r$  corresponds to the area at distance  $r$  from the centre of the polyhedron and  $V_r$  is its respective potential .  $V_r$  was interpolated into the results ( Appendix II ) given by Heine by means of the Lagrangian interpolation formula .

DETERMINATION  
OF EQUIPOTENTIAL SURFACES

$\gamma$	
0.70711	"Caps" subtracted from sphere
0.74162	
0.86605	triangular and square plane base of pyramids
1.00000	square plane bases of pyramids



THE REGION OF "CAPS"

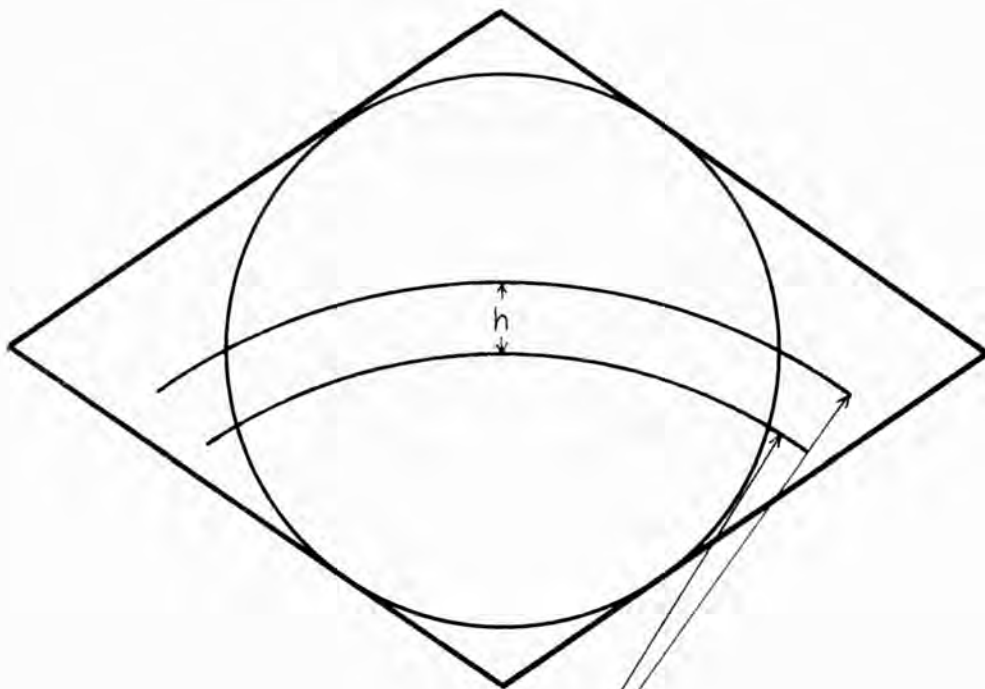


Fig. 6

SQUARE PLANE BASES OF PYRAMIDS

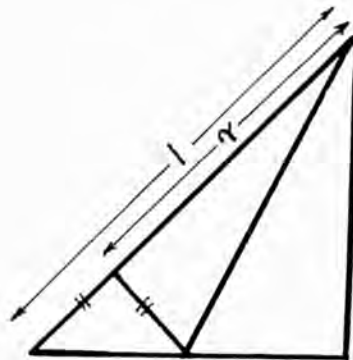
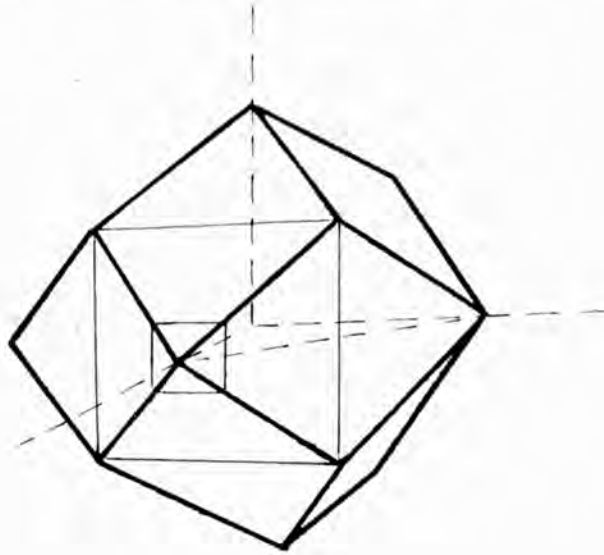


Fig. 7

Area of a small square plane =  $4(1-r)^2$

TRIANGULAR PLANE BASES OF PYRAMIDS

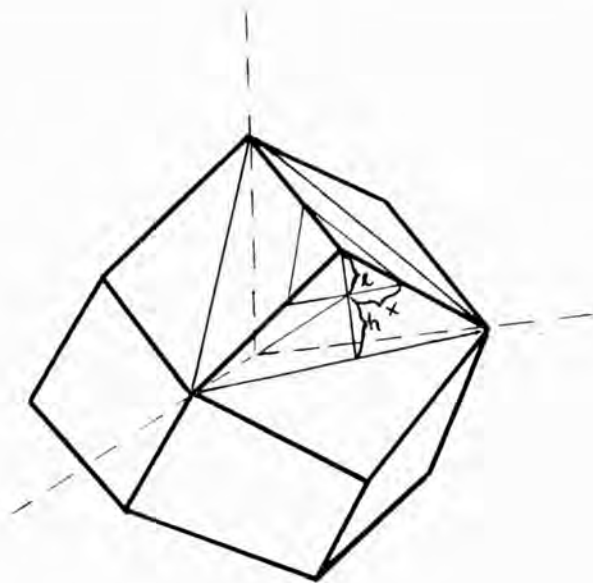


Fig. 8

$$\begin{aligned} \text{Area of a small triangular plane} &= \\ &= 2\sqrt{3} \left\{ \frac{1}{2} - \sqrt{r^2 - \frac{1}{2}} \right\}^2 \end{aligned}$$

DETERMINATION OF CONSTANT POTENTIAL  $V_c$

$V_{Ry}$	$r$	$h$	$A=24\pi rh$	$S=4\pi r^2$	$S-A$	$V_{Ry}(S-A)$
0.21851	0.70711	0		6.28332	6.28332	1.37297
0.19786	0.73329	0.02618	1.44768	6.75704	5.30936	1.05051

		$S_1=24(1-r)^2$	$\frac{1}{2}\sqrt{r^2-\frac{1}{2}}$	$S_2=16\sqrt{3}\{\frac{1}{2}-\sqrt{\cdot}\}$	$S_1+S_2$	$(S_1+S_2)V_{Ry}$
0.18035	0.75948	1.38840	0.22287	6.17653	7.56553	1.36444
0.15867	0.78567	1.10256	0.15751	4.36517	5.46773	0.86757
0.11871	0.81186	0.84960	0.10100	2.79907	3.64867	0.43313
0.08500	0.83805	0.62952	0.05023	1.39205	2.02157	0.17183
0.05394	0.86424	0.44232	0.00311	0.08619	0.05285	0.02851
0.03029	0.89043	0.28824			0.28824	0.00873
0.01371	0.91662	0.16680			0.16680	0.00229
0.00556	0.94280	0.07848			0.07848	0.00044
0.00135	0.96899	0.02304			0.02304	0.00003
					31.38125	5.30045

$$V_c = 0.169 \text{ Ry}$$

LAGRANGIAN INTERPOLATION FORMULA

This approximates ( without remainder term ) a given function by a polynomial .

$$\begin{aligned} f(x) = & \frac{(x-a_2)(x-a_3)\dots(x-a_n)}{(a_1-a_2)(a_1-a_3)\dots(a_1-a_n)} f(a_1) + \\ & + \frac{(x-a_1)(x-a_3)\dots(x-a_n)}{(a_2-a_1)(a_2-a_3)\dots(a_2-a_n)} f(a_2) + \dots \\ & \dots + \frac{(x-a_1)(x-a_2)\dots(x-a_{n-1})}{(a_n-a_1)(a_n-a_2)\dots(a_n-a_{n-1})} f(a_n) + R_n(x) \quad (45) \end{aligned}$$

$$R_n(x) = \frac{(x-a_1)(x-a_2)\dots(x-a_n)}{n!} f''(\xi) \quad (46)$$

In the above expression ,  $a_1, a_2, \dots, a_n$  there are  $n$  arguments or points for which the value of  $f(x)$  is known , with  $f''(\xi)$  as the  $n^{\text{th}}$  derivative of  $f(x)$  at some point  $\xi$  in the interval containing  $a_1, a_2, \dots, a_n$  and  $x$  . The polynomial of degree  $n-1$  , determined by  $n$  entries , will be referred to as an  $n$  - point interpolation polynomial . Only the fourth -

point has been used here . The interpolated Heine **results** (  $V_c$  - Appendix II ) as well as other values are tabulated on page 115-116.

Having ascertained the potential , we now can select  $\gamma$  ( page 89 ) i.e. the energy for which to evaluate the log. derivative .

NUMERICAL INTEGRATION

AS A METHOD OF SOLVING DIFF. EQUATIONS

The evaluation of the logarithmic derivative is obtained by numerical integration . One of the methods of numerical integration of ordinary differential equations consists in evaluating the solution step by step over a series of equal intervals in the independent variable. A step by step solution has to start at some point of the range with definite numerical values of a quantity sufficient to define a solution . We will consider only a solution with the initial conditions for a second order equation with the first derivative absent .

$y'' = f(x, y)$  in which  $f(x, y)$  need not be linear in  $y$  . This is integrated by using the formula of twofold integration from  $y''$  to  $y$  without the intermediate calculation of  $y'$

$$y_1 - 2y_0 + y_{-1} = \int^2 y_0 = (\Delta x)^2 \left[ y_0'' + \frac{1}{12} \Delta^2 y_0'' - \frac{1}{240} \Delta^4 y_0'' \right] + O(\Delta x)^8 \quad (47)$$



the term  $\frac{1}{240} \mathcal{S}^4 y_0''$  in the above expression is negligible, so that the integration formula can be used in the form

$$\mathcal{S}^2 y_0 = (\mathcal{S}x)^2 \left[ y_0'' + \frac{1}{12} \mathcal{S}^2 y_0'' \right] \quad (48)$$

To start the integration, two values of  $y$  are required, and it is advisable to have three to provide a check and to give an indication of the values of  $\mathcal{S}^2 y_0''$ . These initial values are obtained here from a series solution, using the following relations :

$$V = -\left(\frac{26}{r} + C_1 + C_2 r\right) \quad (49)$$

$$\psi = \sum a_n r^n \quad (50)$$

$$\psi'' + \left[ (E+V) - \frac{\ell(\ell+1)}{r^2} \right] \psi = 0 \quad (51)$$

$$\psi = rR$$

for  $\ell=0$  49 and 45 is introduced into 46 to find

$a_2, a_3, a_4$  if  $a_0=0$  and  $a_1=1$  also there is no -ve power ,

$$n=0 \quad a_2 = -13$$

$$n=1 \quad a_3 = \frac{338-(E+C_1)}{6}$$

$$n=2 \quad a_4 = -\frac{[C_2-(E+C_1) + 26 \frac{338-(E+C_1)}{6}]}{12}$$

from this we find that

$$\psi = r - 13r^2 + 68.79667r^3 - 658.9266r^4 \quad (52)$$

$C_1$  and  $C_2$  are found by using Heine values of potential .

If  $\mathcal{S}^2 y''$  is not too large , a good approximation to  $\mathcal{S}^2 y_0$  is  $(\mathcal{S}x)^2 y_0''$  so that 48 reduces to the form below

$$y_1 = 2y_0 - y_{-1} + (\mathcal{S}x)^2 y_0'' \quad (53)$$

Whenever a change of interval length of integration occurred in our case ,there was the usual overlapping between the integration carried out with two different interval lengths. All that was necessary to alter the interval length , was to take two consecutive values of  $y$  and the last value of  $y''$  at the new interval . The smaller the interval  $(\mathcal{S}x)$  taken , the better the estimate of  $\mathcal{S}^2 y''$

however , the interval length  $(\Delta x)$  should be as large as is compatible with the case in the practical numerical working of the integration .

A check carried out on a series of values of  $y$  , was provided by taking and differencing two consecutive values of  $y$  at the start and the end of the interval ( a number of  $y$  values ) respectively . The values of  $(\Delta x)^2 y''$  of this interval were summed up and with the proper sign prefixed , added to the above differences . If the integration is carried out properly , the final result should be zero . The checking intervals also overlapped mutually as the integration was proceeding .

The numerical integration for different values of  $E$  made it possible to evaluate the logarithmic derivative  $\frac{\partial R_e}{\partial r} / R_e$  for certain values of  $\gamma$  which is necessary to calculate the ratio  $\frac{A_0}{B_0}$  required in the surface integral . Using the solution of the radial function eq. 16 we find that

$$\frac{A_0}{B_0} = \frac{n_1(\gamma r_0) - \frac{D}{\gamma} n_0(\gamma r_0)}{\frac{D}{\gamma} j_0(\gamma r_0) + j_1(\gamma r_0)} \quad (54)$$

$$D = \frac{\partial R_0}{\partial \gamma} / R_0 \quad r_0 = \text{radius of inscribed sphere} \cdot$$

These values , together with any intermediate result obtained , have been tabulated on page 89 .

NUMERICAL INTEGRATION RESULTS AND RADICAL EQUATION CONSTANTS

TABLE 7

$\gamma$	$E_{R\gamma}$	$r\psi$	$\frac{d}{dr}(r\psi)$	$\psi$	$\frac{d}{rdr}(r\psi)$	$\frac{\psi}{r}$	$\frac{d\psi}{dr}$	$D = \frac{d^2\psi}{dr^2}$	$A_0/B_0$
	-0.1289	0.153401	0.02037	0.056815	0.007544	0.021043	-0.013499	-0.237596	
	-0.1589	0.157445	0.02571	0.058313	0.009522	0.021597	-0.012075	-0.207072	
0.1	-0.1789	0.159875	0.02926	0.059213	0.010837	0.021931	-0.011094	-0.187358	-91.12626
0.2	-0.2089	0.163926	0.03475	0.060713	0.012870	0.022486	-0.009616	-0.158385	-52.09337
	-0.21727	0.165165	0.03644	0.061172	0.013496	0.022652	-0.009156	-0.149676	
0.6	-0.5289	0.207904	0.09806	0.07700	0.036319	0.028519	0.007800	0.101299	181.69226
0.8	-0.8089	0.249789	0.16455	0.092514	0.060944	0.034264	0.026680	0.288389	17.94810

CALCULATION OF ENERGY  $\Gamma_1$  FOR A1

In the first place , we shall consider the effect of a change of a real  $\gamma$  to an imaginary value in the Bessel functions . As has been already pointed out , the series of the half order Bessel functions converge to relatively simple trigonometric functions , and that is why the trigonometric functions of imaginary angles are here expressed as hyperbolic functions of real angles . This procedure enables us to determine  $f_0 f_1$  , and  $n_0 n_1$  ( for  $i\gamma$  ) .

$$f_0 = \frac{\sinh x}{x}$$

$$n_0 = -i \frac{\cosh x}{x}$$

$$f_1 = i \left\{ \frac{\cosh x}{x} - \frac{\sinh x}{x^2} \right\} \quad n_1 = \frac{\cosh x}{x^2} - \frac{\sinh x}{x} \quad ( 55 )$$

The calculation of the surface integral , however , requires values of the logarithmic derivative of solutions

of the radial differential equation for  $l=0$  .

It is clear from this discussion that the equation 54 must be also approximately modified to fit the present conditions .

$$\frac{A_0}{B_0} = \frac{n_1 - \frac{D}{\gamma} n_0}{\frac{D}{\gamma} j_0 + i j_1} = i \frac{n_1 - \frac{D}{\gamma} n_0}{\frac{D}{\gamma} j_0 - j_1} = i d \quad (56)$$

We may , therefore , write the surface integral

$$\begin{aligned} \int_s &= \frac{A_0^2}{\sqrt{2}} \int_s x j_1 j_0 ds - \frac{B_0^2}{\sqrt{2}} \int_s x n_1 n_0 ds + i \frac{A_0 B_0}{\sqrt{2}} \int_s x \{n_1 j_0 + j_1 n_0\} ds \\ &= \frac{1}{\sqrt{2}} \left[ \frac{A_0^2}{B_0^2} \int_s x j_1 j_0 ds - \int_s x n_1 n_0 ds + i \frac{A_0}{B_0} \int_s x \{n_1 j_0 + j_1 n_0\} ds \right] \\ &= -\frac{1}{\sqrt{2}} \left[ d^2 \int_s x j_1 j_0 ds - \int_s x n_1 n_0 ds + d \int_s x \{n_1 j_0 + j_1 n_0\} ds \right] \quad (57) \end{aligned}$$

so that the  $\left(\frac{1}{\gamma} = X\right)$  integrals then are  $(n_0 - ve)$



$$1) \quad d^2 \int_s x_{j_1 j_0} ds$$

$$2) \quad - \int_s x_{n_1 n_0} ds \quad ( 58 )$$

$$3) \quad d \int_s x \{ n_1 j_0 - j_1 n_0 \} ds$$

The procedure leading to the evaluation of the surface integral for  $\Gamma_1$  A1 is identical with that followed in the case of the empty lattice test .

The manner of tabulation of intermediate values and results is here therefore the same as observed in the case referred to (page 98 -108 ). The stationary value of  $\mathcal{J}=0$  has been found from the graph on page 111 .

DISCUSSION OF THE RESULTS

It is demonstrated in the present work that the constant potential method calculation of electronic structures in monoatomic crystals can be carried out in a systematic way by the use of variational method . However , a reliable approximation of the constant potential must be available .

The present results indicate that the accuracy obtained is not very good . The deviation of the energy calculated here from the true value is attributable to the following facts :

The first and most important one is the application , in the surface integration , of the cubature formula. The error contained in this formula may be as great as 6.5 % ( the empty lattice test results ). To bring it down to about 2% ( as in the case of the least

square method ( Proc. of the Royal Soc. A. vol. 217 p. 71 , 1953 ) or possibly less , the following procedure is recommended : The number of points must exceed 15 and the selection of  $\gamma$  values must never be very close to the stationary point in order to avoid the multiplication of small differences by the large coefficient of the cubature formula. ( Exp. in 15 and 19 integral , for close values of  $\gamma$  , the fifth place beyond the point is uncertain and this has to be multiplied in some places by the constant coefficients  $4 \times 16$  of the cubature formula , shifting the uncertainty much closer to the point ).

Secondly , in the calculation of the constant potential which is , in itself , only an approximation, caps were assumed to be planes , and the separation of the equipotential surface was distorted . However , the total error involved here is not more than  $0.02 R_y$  .

Thirdly , the approximation of the interpolation of intermediate values in the use of Lagrangian coefficients becomes negligible when selected values of  $\gamma$  are not very close to each other. A certain inexact -

itude is also caused by the use of graphs in the reading of the final results ( small number of points page 111) . The value of energy for Al  $\Gamma_1$  , with omission of the additional potential due to the correlation and exchange hole round the electron , is  $-0.19R_{Hy}(\pm 0.01)$ .

Let  $E(k') = \frac{1}{2} (k')^2 - V_{BP}(k') + \text{const.}$

$k' = k + k_m$  where  $k_m$  is  $2\pi$  times the appropriate reciprocal lattice displacement and

$V_{BP}(k')$  Bohm and Pines expression .

The constant in the above equation has been determined by Heine in such a way that the energy of the " free - electron model " equals that obtained in the band structure calculation

$$(V_{BP} = 0.560 \text{ for } k'=0 \quad E(k') = -0.637)$$

This means that the energy calculated here differs from that of Heine by  $1\text{eV}$  ( different zero energy assumption ) so that the validity of the result here can only be verified by finding the separation of the bands .

The advantages of this method can be summarized as follows :

A greater generalization of the problem may be attained by applying the constant potential method in the energy calculation of different crystal type solids as functions of  $K$  , before the application of a mere exact procedure . The calculation of the band structure for a particular ion potential requires only the knowledge of the logarithmic derivative of the radial wave functions (  $D$  ) of different  $\ell$  on the surface of the sphere (  $r_0$  ) . Moreover , once certain " structure constants " in the method have been calculated for a given type of the lattice , they may be used with different potentials without much additional effort .

Thus we may say that this method considerably cuts down the time of the calculation without involving complicated mathematical problems and without introducing any additional approximations than that of the constant potential between the atomic sphere and the polyhedron . This may be , of course , rather

a deviation from the truth , but , in any case ,  
almost all calculations assume a spherical symmetric-  
al potential which is just a rough approximation .

INTERPOLATED BESSEL FUNCTION VALUES  
AND INTERMEDIATE RESULTS



TABLE 8.

N	$\gamma$	$\gamma r$	$X(\frac{\gamma}{r})$	$f_0(\gamma r)$	$f_1(\gamma r)$	$h_0(\gamma r)$	$h_1(\gamma r)$
1	0.10	0.10	0.10	1.00170	0.03300	10.05000	99.49830
	0.20	0.20	0.20	1.00670	0.06690	5.10040	24.49530
	0.60	0.60	0.60	1.06060	0.20811	1.97578	2.23237
	0.80	0.80	0.80	1.11010	0.28416	1.67179	0.97964
2	0.10	0.08839	0.11314	1.00126	0.02987	11.35699	127.45453
	0.20	0.17678	0.22627	1.00518	0.06256	5.74608	31.49818
	0.60	0.53033	0.67882	1.04757	0.18176	2.15708	3.01987
	0.80	0.70711	0.90509	1.08547	0.24766	1.78274	1.43569
3	0.10	0.07906	0.12649	1.00107	0.02597	12.68741	159.43660
	0.20	0.15812	0.25298	1.00447	0.05102	6.41027	39.49233
	0.60	0.47435	0.75893	1.03789	0.16178	2.34981	3.91584
	0.80	0.63247	1.01190	1.06805	0.21934	1.90802	1.94874
4	0.10	0.07289	0.13720	1.00089	0.02432	13.75355	187.57764
	0.20	0.14577	0.27440	1.00356	0.04852	6.93305	46.55695
	0.60	0.43732	0.82320	1.03219	0.14776	2.50803	4.70285
	0.80	0.58309	1.09761	1.05757	0.20119	2.01490	2.39800
5	0.10	0.07071	0.14142	1.00082	0.02375	14.17698	199.45876
	0.20	0.14142	0.28284	1.00335	0.04706	7.14194	49.49974
	0.60	0.42427	0.84852	1.03028	0.14393	2.57231	5.03272
	0.80	0.56569	1.13137	1.06329	0.19470	2.05821	2.58424
6	0.10	0.07181	0.13926	1.00085	0.02404	14.07162	193.32166
	0.20	0.14362	0.27852	1.00346	0.04780	7.03470	47.97760
	0.60	0.43085	0.83555	1.03123	0.14611	2.53960	4.86317
	0.80	0.57447	1.11407	1.05590	0.19793	2.03597	2.48818
7	0.10	0.07395	0.13523	1.00092	0.02459	13.55722	182.19795
	0.20	0.14790	0.27045	1.00367	0.04919	6.83528	45.21102
	0.60	0.44371	0.81135	1.03316	0.15658	2.48504	4.56726
	0.80	0.59161	1.08180	1.05908	0.20470	1.99484	2.31282
8	0.10	0.08004	0.12494	1.00110	0.02627	12.53363	155.58992
	0.20	0.16008	0.24988	1.00460	0.05148	6.32711	38.52001
	0.60	0.48023	0.74964	1.03884	0.16389	2.32712	3.80702
	0.80	0.64031	0.99951	1.06976	0.22228	1.89300	1.88661

TABLE 8.

N	$\gamma$	$\gamma r$	$X(\frac{\gamma}{r})$	$f_0(\gamma r)$	$f_1(\gamma r)$	$n_0(\gamma r)$	$n_1(\gamma r)$
9	0.10	0.08927	0.11202	1.00129	0.03029	11.24639	124.96306
	0.20	0.17854	0.22405	1.00529	0.06376	5.69131	30.87127
	0.60	0.53561	0.67213	1.04850	0.18370	2.14130	2.94937
	0.80	0.71414	0.89618	1.08724	0.25036	1.77279	1.39518
10	0.10	0.08992	0.12061	1.00115	0.02749	12.10019	144.87252
	0.20	0.16583	0.24121	1.00471	0.05427	6.11324	35.85870
	0.60	0.49749	0.72363	1.04177	0.16996	2.26401	3.50910
	0.80	0.66332	0.96484	1.07505	0.23088	1.85158	1.71634
11	0.10	0.07706	0.12978	1.00100	0.02541	13.01332	167.76384
	0.20	0.15411	0.25956	1.00415	0.05118	6.56602	41.60017
	0.60	0.46233	0.77867	1.03596	0.15679	2.39753	4.14975
	0.80	0.61644	1.03822	1.06457	0.21336	1.94033	2.08306
12	0.10	0.07500	0.13333	1.00095	0.02486	13.36834	177.10820
	0.20	0.15000	0.26667	1.00380	0.04980	6.74180	43.94153
	0.60	0.45000	0.80000	1.03410	0.16704	2.46504	4.44377
	0.80	0.60000	1.06667	1.06060	0.20811	1.97578	2.23237
13	0.10	0.08004	0.12494	1.00110	0.02627	12.53363	155.58992
	0.20	0.16008	0.24988	1.00460	0.05148	6.32711	38.52001
	0.60	0.48023	0.74964	1.03884	0.16389	2.32712	3.80702
	0.80	0.64031	0.99951	1.06976	0.22228	1.89300	1.88661
14	0.10	0.08197	0.12200	1.00114	0.02708	12.23971	148.27822
	0.20	0.16394	0.24400	1.00470	0.05324	6.18190	41.69365
	0.60	0.49181	0.73199	1.04082	0.16794	2.28421	3.60369
	0.80	0.65574	0.97578	1.07319	0.22815	1.86476	1.77055
15	0.10	0.08661	0.11547	1.00125	0.02912	11.58835	132.74204
	0.20	0.17321	0.23093	1.00496	0.05967	5.92157	32.82863
	0.60	0.51963	0.69280	1.04563	0.17789	2.19016	3.16920
	0.80	0.69284	0.92373	1.08198	0.24218	1.80384	1.52158

VALUES OF INTEGRALS

The first vertical column represents 15  
points of surface integration and the  
first horizontal the particular integrals  
used.

TABLE 9.

N	$\gamma$	1	2	3
1	0.10	0.00331	-99.99579	9.93358
	0.20	0.01347	-24.98717	4.86359
	0.60	0.13243	-2.64640	1.17388
	0.80	0.25236	-1.31020	0.48995
2	0.10	0.00338	-163.77015	14.39999
	0.20	0.01423	-40.95285	6.26037
	0.60	0.12925	-4.42190	1.88132
	0.80	0.24332	-2.31654	1.01089
3	0.10	0.00329	-255.86864	20.14704
	0.20	0.01297	-64.04359	9.95269
	0.60	0.12743	-6.98328	2.79594
	0.80	0.23706	-3.76249	1.68263
4	0.10	0.00334	-353.95713	25.71266
	0.20	0.01336	-88.57129	12.72840
	0.60	0.12556	-9.70955	3.69094
	0.80	0.23354	-5.30336	2.33865
5	0.10	0.00336	-399.89686	28.18297
	0.20	0.01336	-99.99078	13.95235
	0.60	0.12583	-10.98470	4.05570
	0.80	0.23422	-6.01766	2.65541
6	0.10	0.00335	-378.83506	26.89775
	0.20	0.01336	-94.00273	13.31530
	0.60	0.12589	-10.31947	3.88029
	0.80	0.23283	-5.64372	2.47800
7	0.10	0.00333	-334.03079	24.61621
	0.20	0.01335	-83.57716	12.18126
	0.60	0.13125	-9.20868	3.51282
	0.80	0.23452	-4.99111	2.20808
8	0.10	0.00329	-243.64604	19.41965
	0.20	0.01292	-60.90084	9.58827
	0.60	0.12763	-6.64135	2.67884
	0.80	0.23767	-3.56960	1.59666

TABLE 9.

N	$\gamma$	1	2	3
9	0.10	0.00340	-157.43096	13.97827
	0.20	0.01436	-39.36513	6.87199
	0.60	0.12946	-4.24483	1.81412
	0.80	0.24394	-2.21658	0.96166
10	0.10	0.00332	-211.42696	17.45305
	0.20	0.01315	-52.87633	8.61019
	0.60	0.12813	-5.74898	2.36691
	0.80	0.23948	-3.06620	1.36782
11	0.10	0.00330	-283.33132	21.75125
	0.20	0.01334	-70.89818	10.75533
	0.60	0.12648	-7.74711	3.05478
	0.80	0.23582	-4.19630	1.87250
12	0.10	0.00331	-315.67766	23.59196
	0.20	0.01333	-78.99966	11.67289
	0.60	0.13819	-8.76326	3.34683
	0.80	0.23544	-4.70473	2.08691
13	0.10	0.00329	-243.64604	19.41965
	0.20	0.01292	-60.90084	9.58827
	0.60	0.12763	-6.64135	2.67884
	0.80	0.23767	-3.56960	1.59666
14	0.10	0.00331	-221.41645	18.07013
	0.20	0.01305	-62.89002	10.14076
	0.60	0.12795	-6.02544	2.46474
	0.80	0.23892	-3.22168	1.43897
15	0.10	0.00337	-177.62345	15.30792
	0.20	0.01385	-44.89165	7.53712
	0.60	0.12887	-4.80877	2.02589
	0.80	0.24205	-2.53535	1.11722

THE SURFACE INTEGRAL  
IN THE CUBATURE FORM

In tables 10,11,12 and 13 the first column represents the points on the surface of integration and in the last the cubature coefficients by which the remaining column are multiplied.



TABLE 10.

N	A. <sup>2</sup>	B. <sup>2</sup>	A.B.	
1/2	0.00166	49.99790	4.96679	
	0.00166	49.99790	4.96679	1
2	0.01352	655.08060	57.59996	
	0.00338	163.77015	14.39999	4
3	0.00658	511.73728	40.29408	
	0.00329	255.86864	20.14704	2
4	0.01336	1415.82852	102.85064	
	0.00334	353.95713	25.71266	4
5	0.00336	399.89686	28.18297	
	0.00336	399.89686	28.18297	1
6	0.01340	1515.34024	107.59100	
	0.00335	378.83506	26.89775	4
7	0.05328	5344.49264	393.85936	
	0.00333	334.03079	24.61621	16
8	0.02632	1949.16832	155.35720	
	0.00329	243.64604	19.41965	8
9/2	0.02720	1259.44768	111.82624	
	0.00170	78.71548	6.98914	16
10/2	0.01328	845.70784	69.81220	
	0.00332	211.42696	17.45305	4
11	0.02640	2266.65056	174.01000	
	0.00330	283.33132	21.75125	8
12	0.00662	631.35532	47.18392	
	0.00331	315.67766	23.59196	2
13	0.01316	974.58416	77.67860	
	0.00329	243.64604	19.41965	4
14/2	0.02656	1771.33168	144.56112	
	0.00166	110.70823	9.03507	16
15/2	0.00169	88.81173	7.65396	
	0.00169	88.81173	7.65396	1
	0.24539	19679.43133	1523.42804	

$$\gamma = 0.10$$



TABLE 11.

N	$A_0^2$	$B_0^2$	$A_0 B_0$	
1/2	0.00674	12.49359	2.43180	
	0.00674	12.49359	2.43180	1
2	0.05692	163.81140	25.04148	
	0.01423	40.95285	6.26037	4
3	0.02594	128.08706	19.90538	
	0.01297	64.04353	9.95269	2
4	0.05344	354.28516	50.91360	
	0.01336	88.57129	12.72840	4
5	0.01336	99.99078	13.95235	
	0.01336	99.99078	13.95235	1
6	0.05344	376.01092	53.26120	
	0.01336	94.00273	13.31530	4
7	0.21360	1337.23456	194.90016	
	0.01335	83.57716	12.18126	16
8	0.10336	487.20672	76.70616	
	0.01292	60.90084	9.58827	8
9/2	0.11488	314.92112	54.97600	
	0.00718	19.68257	3.43600	16
10/2	0.05260	211.50532	34.44076	
	0.01315	52.87633	8.61019	4
11	0.10672	567.18544	86.04264	
	0.01334	70.89818	10.75533	8
12	0.02666	157.99932	23.34578	
	0.01333	78.99966	11.67289	2
13	0.05168	243.60336	38.35308	
	0.01292	60.90084	9.58827	4
14/2	0.10448	503.12016	81.12608	
	0.00653	31.44501	5.07038	16
15/2	0.00693	22.44583	3.76856	
	0.00693	22.44583	3.76856	1
	0.99075	4979.90074	759.16503	

$$\gamma = 0.20$$

TABLE 12.

N	$A_0^2$	$B_0^2$	$A_0 B_0$	
1/2	0.06622	1.32320	0.58694	
	0.06622	1.32320	0.58694	1
2	0.51700	17.68760	7.52528	
	0.12925	4.42190	1.88132	4
3	0.25486	13.96656	5.59188	
	0.12743	6.98328	2.79594	2
4	0.50224	38.83820	14.76376	
	0.12556	9.70955	3.69094	4
5	0.12583	10.98470	4.05570	
	0.12583	10.98470	4.05570	1
6	0.51436	41.27788	15.52116	
	0.12589	10.31947	3.88029	4
7	2.10000	147.33888	56.20512	
	0.13125	9.20868	3.51282	16
8	1.02104	53.13080	21.43072	
	0.12763	6.64135	2.67884	8
9/2	1.03568	33.95872	14.51296	
	0.06473	2.12242	0.90706	16
10/2	0.51252	22.99592	9.46764	
	0.12813	5.74898	2.36691	4
11	1.01184	61.97688	24.43824	
	0.12648	7.74711	3.05478	8
12	0.27638	17.52652	6.69366	
	0.13819	8.76326	3.34683	2
13	0.51052	26.56540	10.71536	
	0.12763	6.64135	2.67884	4
14/2	1.02368	48.20352	19.71792	
	0.06398	3.01272	1.23237	16
15/2	0.06444	2.40439	1.01295	
	0.06444	2.40439	1.01295	1
	9.53661	538.17917	212.23929	

$$\gamma = 0.60$$

TABLE 13.

N	$A_0^2$	$B_0^2$	$A_0 B_0$	
1/2	0.12618	0.65510	0.24498	
	0.12618	0.65510	0.24498	1
2	0.97328	9.26616	4.04356	
	0.24332	2.31654	1.01089	4
3	0.47412	7.52498	3.36526	
	0.23706	3.76249	1.68263	2
4	0.93416	21.21344	9.35460	
	0.23354	5.30336	2.33865	4
5	0.23422	6.01760	2.65541	
	0.23422	6.01760	2.65541	1
6	0.93132	22.57488	9.91200	
	0.23283	5.64372	2.47800	4
7	3.75232	79.85776	35.32928	
	0.23452	4.99111	2.20808	16
8	1.90136	28.55680	12.77328	
	0.23767	3.56960	1.59666	8
9/2	1.95152	17.73264	7.69328	
	0.12197	1.10829	0.48083	16
10/2	0.95792	12.26480	5.47128	
	0.23948	3.06620	1.36782	4
11	1.88656	33.57040	14.98000	
	0.23582	4.19630	1.87250	8
12	0.47088	9.40946	4.17382	
	0.23544	4.70473	2.08691	2
13	0.95068	14.27840	6.38664	
	0.23767	3.56960	1.59666	4
14/2	1.91136	25.77344	11.51184	
	0.11946	1.61084	0.71949	16
15/2	0.12103	1.26768	0.55861	
	0.12103	1.26768	0.55861	1
	17.57691	289.96354	128.45384	

$$\gamma = 0.80$$

SURFACE INTEGRALS

$$\gamma = 0.1$$

$$\begin{aligned} -I_2 &= (91.12626)^2 \times 0.24539 - 19679.43133 - 91.12626 \times 1529.68650 \\ &= -147036.32365 \end{aligned}$$

$$I_2 = 147036.32365$$

$$\gamma = 0.2$$

$$\begin{aligned} -I_2 &= (52.09337)^2 \times 0.99075 - 4979.90074 - 52.09337 \times 759.16503 \\ &= -41838.74824 \end{aligned}$$

$$41838.74824$$

$$\gamma = 0.6$$

$$\begin{aligned} -I_2 &= (181.69226)^2 \times 9.53661 - 538.17917 + 181.69226 \times 212.23929 \\ &= 352847.36397 \end{aligned}$$

$$I_2 = -352847.36397$$

$$\gamma = 0.8$$

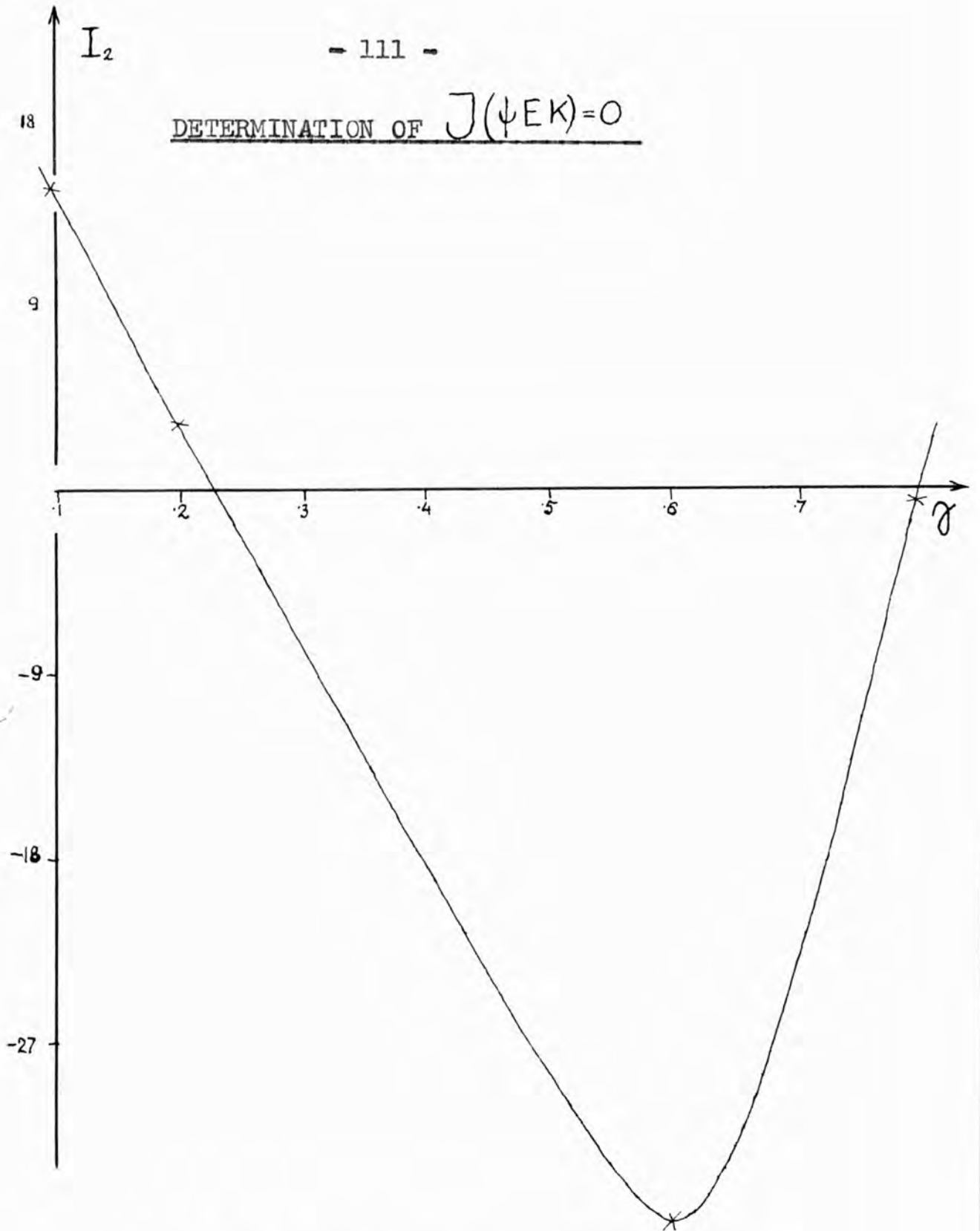
$$\begin{aligned} -I_2 &= (17.94810)^2 \times (17.57691) - 289.96354 + 17.94810 \times 128.45384 \\ &= 7677.66425 \end{aligned}$$

$$I_2 = -7677.66425$$

SURFACE INTEGRALS

$\theta$	$I_2$
0.1	147036.32365
0.2	41838.74824
0.6	-352847.36397
0.8	- 7677. 66425

DETERMINATION OF  $J(\psi EK)=0$



$I_2$  is plotted against corresponding values of  $\gamma$

APPENDIX I.

X	$f_0$ +ve	$f_1$ +ve i	$n_0$ -ve i	$n_1$ +ve
0.01	1.00000	0.00500	100.00500	9999.50000
0.02	1.00000	0.01000	50.01000	2499.50000
0.03	1.00010	0.01163	33.34830	1110.61000
0.04	1.00020	0.01500	25.02000	624.49980
0.05	1.00040	0.01700	20.02500	399.49960
0.06	1.00060	0.02003	16.69670	277.27773
0.07	1.00080	0.02356	14.32070	203.58034
0.08	1.00110	0.02625	12.54000	155.74890
0.09	1.00130	0.03054	11.15610	122.95426
0.10	1.00170	0.03300	10.05000	99.49830
0.11	1.00200	0.03691	9.14600	82.14356
0.12	1.00240	0.04007	8.39340	68.94260
0.13	1.00280	0.04355	7.75740	58.66951
0.14	1.00330	0.04657	7.21300	50.52099
0.15	1.00380	0.04980	6.74180	43.94153
0.16	1.00460	0.05145	6.33020	38.55915
0.17	1.00480	0.05691	5.96750	34.09814
0.18	1.00540	0.06458	5.64680	30.36571
0.19	1.00610	0.06314	5.35840	27.19601
0.20	1.00670	0.06690	5.10040	24.49530
0.21	1.00740	0.07016	4.86730	22.17022
0.22	1.00810	0.07363	4.65590	20.15508
0.23	1.00880	0.07801	4.46410	18.40033
0.24	1.00970	0.08002	4.28710	16.85322
0.25	1.01040	0.08404	4.12564	15.49216
0.26	1.01130	0.08727	3.97689	14.28443
0.27	1.01220	0.09063	3.83952	13.20824
0.28	1.01330	0.09325	3.71218	12.24449
0.29	1.01410	0.09741	3.59431	11.38007
0.30	1.01510	0.10080	3.48447	10.36497
0.31	1.01610	0.10433	3.38207	9.89380
0.32	1.01720	0.10763	3.28638	9.25274
0.33	1.01830	0.11106	3.19682	8.66903



APPENDIX I.

$x$	$f_0$ +ve	$f_1$ +ve i	$n_0$ -ve i	$n_1$ +ve
0.34	1.0194	0.11458	3.11282	8.13595
0.35	1.0205	0.11823	3.03394	7.64790
0.36	1.0217	0.12166	2.95972	7.19974
0.37	1.0230	0.12494	2.88981	6.78730
0.38	1.0242	0.12861	2.82387	6.40704
0.39	1.0255	0.13210	2.76159	6.05550
0.40	1.0269	0.13543	2.70268	5.72980
0.41	1.0283	0.13885	2.64690	5.42615
0.42	1.0297	0.14238	2.59405	5.14661
0.43	1.0311	0.14600	2.54391	4.88497
0.44	1.0326	0.14948	2.49630	4.64081
0.45	1.0341	0.16704	2.46504	4.44377
0.46	1.0356	0.15670	2.40800	4.19918
0.47	1.0372	0.16021	2.36702	3.99901
0.48	1.0388	0.16381	2.32798	3.81116
0.49	1.0405	0.16729	2.29076	3.63452
0.50	1.0422	0.17086	2.25526	3.46832
0.51	1.0439	0.17449	2.22135	3.31169
0.52	1.0457	0.17802	2.18898	3.16388
0.53	1.0475	0.18164	2.15806	3.02431
0.54	1.0493	0.18533	2.12848	2.89233
0.55	1.0512	0.18900	2.10027	2.76747
0.56	1.0531	0.19257	2.07311	2.64888
0.57	1.0550	0.19631	2.04719	2.53656
0.58	1.0570	0.19995	2.02236	2.42983
0.59	1.0588	0.20400	1.99858	2.32862
0.60	1.0606	0.20811	1.97578	2.23237
0.61	1.0632	0.21097	1.95392	2.13995
0.62	1.0653	0.21474	1.93297	2.05239
0.63	1.0675	0.21842	1.91286	1.96879
0.64	1.0697	0.22216	1.89358	1.88902
0.65	1.0719	0.22598	1.87506	1.81281
0.66	1.0742	0.22972	1.85730	1.73989
0.67	1.0767	0.23323	1.84025	1.66994

APPENDIX I.

$X$	$f_0$ +ve	$f_1$ +ve	$n_0$ -ve	$n_1$ +ve
0.68	1.0789	0.23728	1.82390	1.60331
0.69	1.0813	0.24109	1.80819	1.53927
0.70	1.0837	0.24496	1.79310	1.47787
0.71	1.0862	0.24876	1.77862	1.41890
0.72	1.0887	0.25263	1.76471	1.36229
0.73	1.0912	0.25656	1.75136	1.30792
0.74	1.0938	0.25435	1.73854	1.25558
0.75	1.0964	0.26437	1.72624	1.20525
0.76	1.0991	0.26825	1.71443	1.15673
0.77	1.1018	0.27219	1.70310	1.11002
0.78	1.1045	0.26524	1.68127	1.05097
0.79	1.1073	0.28015	1.68180	1.02156
0.80	1.1101	0.28416	1.67179	0.97964
0.81	1.1130	0.28813	1.66220	0.93910
0.82	1.1159	0.29216	1.65301	0.89997
0.83	1.1188	0.29624	1.64419	0.86215
0.84	1.1218	0.30028	1.63576	0.82553
0.85	1.1248	0.30439	1.62768	0.79012
0.86	1.1279	0.30844	1.61995	0.75576
0.87	1.1310	0.31256	1.61256	0.72252
0.88	1.1342	0.31664	1.60550	0.69023
0.89	1.1373	0.32088	1.59875	0.65905
0.90	1.1406	0.32499	1.59232	0.62864
0.91	1.1438	0.32926	1.58618	0.60268
0.92	1.1472	0.33337	1.58033	0.57055
0.93	1.1505	0.33766	1.57476	0.54279
0.94	1.1539	0.34192	1.56947	0.51575
0.95	1.1574	0.34613	1.56445	0.48939
0.96	1.1608	0.35051	1.55968	0.46387
0.97	1.1644	0.35524	1.55565	0.43936
0.98	1.1679	0.35917	1.55091	0.41466
0.99	1.1715	0.36355	1.54688	0.33101
1.00	1.1752	0.36788	1.54308	0.36788

APPENDIX II.

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$r$	$V$	$r$	$V$	$r$	$V$
0.005	5129.2	0.19	81.87895	0.42	24.23810
0.01	2529.0	0.195	79.24829	0.43	23.26047
0.015	1662.533	0.20	76.89500	0.44	22.33864
0.02	1229.6	0.205	74.46681	0.45	21.47333
0.025	970.04	0.210	72.10476	0.46	20.65217
0.03	797.2667	0.215	69.83492	0.47	19.88723
0.035	674.0571	0.22	67.65000	0.48	19.14792
0.04	581.8250	0.225	65.55270	0.49	18.45714
0.045	510.3111	0.23	63.53913	0.50	17.80600
0.05	453.2000	0.235	61.60735	0.51	17.18800
0.055	406.6546	0.24	59.75417	0.52	16.60448
0.06	368.0333	0.245	57.97669	0.53	16.05372
0.065	335.4462	0.25	56.27200	0.54	15.53402
0.07	307.6286	0.255	54.63762	0.55	15.04364
0.075	283.6267	0.26	53.06923	0.56	14.57769
0.08	262.7250	0.265	51.56242	0.57	14.13844
0.085	244.400	0.27	50.11482	0.58	13.72495
0.09	228.1889	0.275	48.72312	0.59	13.33634
0.095	213.7474	0.28	47.38571	0.60	12.97167
0.10	200.86	0.285	46.10083	0.61	12.62403
0.105	189.44732	0.29	44.86555	0.62	12.30003
0.11	179.16364	0.295	43.67728	0.63	12.00019
0.115	169.57628	0.30	42.53333	0.64	11.72512
0.12	160.86667	0.305	41.43068	0.65	11.47539
0.125	153.18678	0.31	40.36774	0.66	11.29090
0.13	146.19231	0.315	39.34223	0.67	11.12307
0.135	139.67945	0.32	38.35313	0.68	10.96269
0.14	133.37857	0.325	37.39920	0.69	10.80045
0.145	126.83179	0.33	36.47879	0.70	10.62714
0.15	120.4000	0.34	34.73235	0.75	9.27067
0.155	114.31111	0.35	33.10286	0.80	6.67625
0.16	108.50625	0.36	31.57778	0.85	4.78471
0.165	102.96672	0.37	30.15135	0.90	3.89111
0.17	97.80000	0.38	28.81579	0.95	3.81053
0.175	93.11343	0.39	27.56154	1.00	3.57400
0.18	88.88889	0.40	26.38250	1.05	3.29905
0.185	85.13846	0.41	25.27805	1.10	3.03727

APPENDIX II

$\gamma$	$V$
1.15	2.78696
1.20	2.55667
1.25	2.34400
1.30	2.14923
1.35	1.91111
1.40	1.81000
1.45	1.66138
1.50	1.52333
1.55	1.397728
1.60	1.28250
1.65	1.176436
1.70	1.07882
1.75	0.988624
1.80	0.90556
1.85	0.829048
1.90	0.75895
2.00	0.63700
2.1	0.53524
2.2	0.45227
2.3	0.38217
2.4	0.32292
2.5	0.27880
2.6	0.24385
2.7	0.21852
2.8	0.19786

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