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Energy Bands of Ferromagnetic Nickel.

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ABSTRACT

The tight binding method has been employed to calculate energy bands in ferromagnetic nickel. The basis set consisted of atomic wave functions for the 1s, 2s, 3s, 4s, 2p, 3p, and 4p states, expressed as linear combinations of Gaussian orbitals, and five individual Gaussian orbitals for each 3d state. The Coulomb part of the crystal potential was constructed from a superposition of overlapping neutral atom charge densities, the atoms being in the $3d^9 4s^1$ configuration. The "$X\alpha$" method of Slater et al was used to construct an exchange potential. Energy levels were calculated at 1505 points in 1/48'th of the Brillouin zone. The results are generally in good agreement with those obtained from other first principles calculations. The properties of several positions of the Fermi surface are determined and compared with experiment. The spin splitting of the d bands is calculated to be about 0.8 ev.

CHAPTER I

Introduction

The relation between band structure and ferromagnetism has long presented a challenge to the theory of solids. The study of the properties of nickel has been of considerable importance for the theory of ferromagnetism, since it appears to be the simpliest of the 3d elemental ferromagnets. However, due to the complexity of band structure investigations, it is necessary to make certain approximations to overcome the mathematical difficulties involved.

One approximation is energy band theory, also called the one electron model. Here, one considers the energy states of a single electron in a rigid, infinite, periodic lattice. The basic problem is to solve the one electron Schrodinger equation

$$H \psi_k = E_k \psi_k \tag{1.1}$$

where H is the Hamiltonian operator, and the wave functions ψ_k are assumed to obey the Bloch condition. This condition is that

$$\psi_k(\underline{r}-\underline{R}_\mu) = e^{-i\underline{k}\cdot\underline{R}_\mu}\, \psi_k(\underline{r}) \tag{1.2}$$

where $\underline{R}_\mu$ is a direct lattice vector and $\underline{k}$ is a reciprocal lattice vector (Bloch, 1928). Within this approximation, many techniques have been developed to obtain energy bands. These various methods attack the problem by expanding the wave function in terms of some known set of functions, such as plane waves, spherical waves, Hartree-Fock atomic wave functions, or combinations of these.

Some of the more important calculations of the band structure of nickel used the Augmented Plane Wave (APW) method (Hanus, 1962; Mattheiss, 1964; Snow et al, 1966; Connolly, 1967; Zornberg, 1970), the Green's function method (Yamashita et al, 1963; Wakoh and Yamashita, 1964; Wakoh, 1965), or the combined interpolation scheme (Hodges et al, 1966; Mueller, 1967; Ruvalds and Falicov, 1968; Zornberg, 1970; Tyler, Norwood, and Fry, 1970; Callaway and Zhang, 1970). These calculations have either been semi-empirical in nature, or have used a "muffin-tin" form of crystal potential. The "muffin-tin" potential consists of a spherically symmetric potential of some radius R_o, placed on each atomic site, and a constant potential between these spheres. The adequacy of approaches based on approximations in which the crystal potential at each atomic site is spherically symmetric in applications to d bands is questionable. These methods also neglect crystal field effects which are small but not entirely negligible (Callaway and Edwards, 1960). Specifically, predictions of the Fermi surface in nickel depend sensitively on the position of the levels X_5 and X_2 at the center of a square face of the

Brillouin zone. The separation of these levels will be influenced by the presence of a term in the crystal potential around each atom having cubic, rather than spherical symmetry as found in the "muffin-tin" potential.

The present work applies the tight binding method to the band structure of nickel. Some preliminary work using the tight binding method has been done by Fletcher and Wohlfarth (1951), Yamashita et al (1963), and Callaway et al (1971). We have decided to apply the tight binding method as improved by Lafon and Lin (1966) in which they have eliminated the three center integrals normally encountered in tight binding by expressing the crystal potential in the form of a Fourier series over the reciprocal lattice vectors. The specific techniques will be dealt with in detail in later sections of this dissertation. In its present form, the method seems to be as accurate as other methods, and in addition does not necessarily incorporate restrictive assumptions about the symmetry of the crystal potential.

The elements of the Hamiltonian and overlap matrices are only dependent on the reciprocal lattice vector, $\underline{k}$, so that all the energy values can be found by a standard diagonalization procedure for each $\underline{k}$. The size of the matrices which must be considered is small enough (here 38 x 38) so that energies can be obtained at a moderate number of general points in the Brillouin zone without an unduly large expenditure of computer time. In fact, the present calculation determined energy levels at 1505 points in 1/48'th of the Brillouin zone in each of the calculations for the up-spin and down-spin band structures of nickel.

This investigation was based on an assumed crystal potential constructed from a superposition of overlapping neutral atom charge densities, the atoms being in the $3d^9 4s^1$ configuration and placed on the sites of a face-centered cubic lattice. The exchange potential was included according to the "$X\alpha$" method of Slater et al (1969) with a spin dependent charge density. This prescription was also used to consider the exchange splitting of the energy bands in the ferromagnetic state by assigning a predetermined electron occupation to the spin dependent charge densities. However, spin orbit coupling was neglected in this work.

The results obtained are compared with those of other methods and with available experimental data. Cross sectional areas are presented for significant sections of the Fermi surface. In general, the results demonstrate that the tight binding method can yield a band structure for a transition metal at least comparable in accuracy to those obtained by other methods of band structure calculations. The agreement with experiment is satisfactory, although not as good as can be obtained by semi-empirical interpolation schemes which have been designed to enable an accurate fit to experimental data. At this point, one must keep in mind the fact that this work is a first principles calculation and does not have a fit to experimental data built in. The characteristics of the present form of the tight binding method are classified by this investigation and the requirements for successful application become apparent.

CHAPTER II

The Tight Binding Method

The tight binding or LCAO (Linear Combination of Atomic Orbitals) was first proposed by Bloch in 1928. Until recently, however, use of the method had largely been restricted either to calculations of a highly empiricalnature or to ones in which it serves as an interpolation scheme after energy bands have been calculated at symmetry points by other methods. The technique has been improved recently by Lafon and Lin (1966) and this, together with the increased efficiency of modern computers has made the tight binding approximation an effective tool for calculating energy bands.

We begin with a set of localized basis functions $u_j(\underline{r})$, which, for convenience, will be assumed normalized, but need not be orthogonal. In conventional descriptions of the tight binding method, the u_j's are chosen to be the one-electron wave functions for each of the electronic states of the free atom of which the crystal is composed. For nickel, j = 1s, 2s, 3s, 4s, 2p, 3p, 4p, and 3d. This procedure is not necessary and may be too restrictive. In this work, some of the u_j's will be atomic functions, others will be individual localized (Gaussian type) orbitals.

In the first step, the one-electron wave functions, $\phi_j(\underline{k},\underline{r})$, of the electron in the crystal are constructed by taking linear combinations of the $u_j(\underline{r})$. These wave functions must satisfy Bloch's theorem for wave vector $\underline{k}$ and are written as

$$\phi_j(\underline{k},\underline{r}) = \frac{1}{\sqrt{N}} \sum_{\mu} e^{i\underline{k}\cdot\underline{R}_\mu} u_j(\underline{r}-\underline{R}_\mu) \qquad (2.1)$$

where N is the number of atoms in the crystal and $\underline{k}$ is a reciprocal lattice vector.

For convenience, we restrict our attention to a crystal with one atom per unit cell, the direct lattice vectors being denoted by $\underline{R}_\mu$. These Bloch functions will be the basis set required in the Hamiltonian and overlap matrices. The set consisting of only the atomic states does not form a complete set, so an expansion of the wave functions using this set as a basis does not lead to an exact solution of the Schrodinger equation. However, the inclusion of all the bound states and excited states can be expected to yield a good approximation to the actual wave function. Since atomic states on different atoms are not orthogonal, the secular determinant has the form

$$\left| H_{ij}(\underline{k}) - E_{k} S_{ij}(\underline{k}) \right| = 0 \qquad (2.2)$$

where H_{ij} and S_{ij} are the matrix elements of the Hamiltonian and of unity with respect to the basis of Bloch functions formed from atomic functions having symmetry properties i and j, respectively.

The present approach differs from more conventional applications of the tight binding method in the treatment of the Hamiltonian. If the crystal potential $V_c(\underline{r})$ is expressed as the sum of individual atomic potentials $V_A(\underline{r} - R_\mu)$, one finds it necessary to compute three center integrals of the form

$$\int u_i(\underline{r})\, V_A(\underline{r}-\underline{R}_\mu)\, u_j(\underline{r}-\underline{R}_\nu)\, d^3r \quad . \tag{2.3}$$

The computation of integrals of this type has been a major obstacle to quantitative development of the tight binding method. Instead of expressing the crystal potential as a sum of atomic potentials, we will use a Fourier representation

$$V_c(\underline{r}) = \sum_s V(\underline{K}_s)\, e^{i\underline{K}_s\cdot\underline{r}} \tag{2.4}$$

in which the $\underline{K}_s$ are reciprocal lattice vectors. We note that each term in the sum, as well as the complete potential, is unchanged by displacement through a direct lattice vector. For this reason, three center integrals do not appear.

Let T denote the kinetic energy term in the Hamiltonian. The matrix elements of the Hamiltonian are

$$\begin{aligned} H_{jn}(\underline{k}) &= \int \phi_j(\underline{k},\underline{r})\left[T + V_c(\underline{r})\right] \phi_n(\underline{k},\underline{r})\, d^3r \\ &= \sum_\mu e^{i\underline{k}\cdot\underline{R}_\mu}\left[T_{jn}(\underline{R}_\mu) + \sum_s V(\underline{K}_s)\, S_{jn}(\underline{k},\underline{K}_s)\right] \quad . \end{aligned} \tag{2.5}$$

The $S_{jn}(k,K_s)$ can be expressed as

$$S_{jn}(\underline{k},\underline{K}_s) = \sum_{\mu} e^{i\underline{k}\cdot\underline{R}_\mu} S_{jn}(\underline{K}_s,\underline{R}_\mu), \qquad (2.6)$$

in which

$$S_{jn}(\underline{K}_s,\underline{R}_\mu) = \int u_j(\underline{r}) e^{i\underline{K}_s\cdot\underline{r}} u_n(\underline{r}-\underline{R}_\mu)\, d^3r \qquad (2.7)$$

The elements of the overlap matrix can be determined from (2.6) simply by setting K=0. The quantity $T_{jn}(\underline{R}_\mu)$ is a matrix element of the kinetic energy operator. In a crystal with a center of inversion, it is sufficient to consider integrals of the form (2.7) with $\cos(\underline{K}_s\cdot\underline{r})$ replacing $e^{i\underline{K}_s\cdot\underline{r}}$. The analytical expressions for $S_{ij}(\underline{K},\underline{R})$ are given in Appendix A. Once these expressions are evaluated, the summation over $\underline{R}_\mu$ indicated in equation (2.5) and the diagonalization of the secular equation (2.2) is performed by the computer program listed in Appendix B.

Equation (2.5) may be written in an alternative manner

$$H_{ij}(\underline{k}) = \sum_{\mu} e^{i\underline{k}\cdot\underline{R}_\mu} E_{ij}(\underline{R}_\mu) \qquad (2.8)$$

in which

$$E_{ij}(\underline{R}_\mu) = T_{ij}(\underline{R}_\mu) + V_{ij}(\underline{R}_\mu), \qquad (2.9)$$

and $V_{ij}(\underline{R}_u)$ is given by

$$V_{ij}(\underline{R}_u) = \sum_s V(\underline{K}_s)\ S_{ij}(\underline{K}_s, \underline{R}_u) \ . \qquad (2.10)$$

The fundamental computational problem in the present approach to the tight binding method is the calculation of the type $S_{ij}(\underline{K},\underline{R})$ appearing in (2.6). A printout of the computer program which computes the d-d symmetry integrals is given in Appendix B. A very large number of such integrals are required (of the order 10^7). For this reason, it is essential to simplify the determination of these quantities as much as possible. To this end, we have decided to work with Gaussian type orbitals (GTO) as suggested by Chaney et al (1970). Gaussian type orbitals are of the form $e^{-\alpha r^2}$. Radial components of atomic wave functions formed by linear combinations of GTO's are written as

$$R_{nl}(\underline{r}) = \sum_i C_{nli}\ N_{li}\ r^{l-1} e^{-\alpha_{li} r^2} \qquad (2.11)$$

where n is the principle quantum number, and l is the symmetry type (s,p,d). The index i indicates the numbers of GTO's used for each electronic state (14 for s, 11 for p, and 5 for d). The value of C_{nli} and α_{ni} of these one-electron wave functions are given by Wachters (1970). The N_{li} is a constant which normalizes each GTO and is given as

$$N_{\ell i} = \left[\sqrt{\frac{2}{\pi}} \; \frac{2^{2\ell+1} \alpha_{\ell i}^{\ell+\frac{1}{2}}}{(2\ell-1)!!} \right]^{\frac{1}{2}} \qquad (2.12)$$

where ℓ = 1, 2, 3 (s, p, d). The advantage of such orbitals is that analytic expressions can be obtained for all of the $S_{jn}(\underline{K}, \underline{R})$.

For example, if j and n both denote s type symmetry, then the expression (2.7) can be written

$$S_{jn}(\underline{K}, \underline{R}) = \langle 1s(\underline{A}) | \cos(\underline{k} \cdot \underline{r}_c) | 1s(\underline{B}) \rangle \qquad (2.13)$$

where 1s($\underline{A}$) denotes an s-type orbital on lattice site $\underline{A}$ (usually taken as the origin as in (2.7)), 1s($\underline{B}$) denotes an orbital on site $\underline{B}$, and $\underline{r}_c$ is the radial vector measured from any given lattice site of the crystal. Hence one can write

$$\langle 1s(\underline{A}) | \cos(\underline{k} \cdot \underline{r}_c) | 1s(\underline{B}) \rangle = \int e^{-(\alpha_1 r_A^2 + \alpha_2 r_B^2)} \cos(\underline{k} \cdot \underline{r}_c) d\tau \qquad (2.14)$$

where $d\tau$ denotes all space and $\underline{r}_A = (\underline{r} - \underline{R}_A)$. The product of two Gaussian orbitals situated at centers $\underline{A}$ and $\underline{B}$ is proportional to a third Gaussian orbital situated at a point $\underline{D}$ along the line $\underline{AB}$, that is,

$$e^{(-\alpha_1 r_A^2 - \alpha_2 r_B^2)} = e^{-\left(\frac{\alpha_1 \alpha_2 r_{AB}^2}{\alpha_1 + \alpha_2}\right)} e^{-(\alpha_1 + \alpha_2) r_D^2} \qquad (2.15)$$

where $\underline{r}_{AB}$ is the distance between the two centers, and $\underline{r}_D$ is the radius vector originated from $\underline{D}$. The coordinates of $\underline{D}$ are related to those of $\underline{A}$ and $\underline{B}$ as

$$D_i = (\alpha_1 A_i + \alpha_2 B_i)/(\alpha_1 + \alpha_2) \; ; \; i = x, y, \text{or } z \, . \qquad (2.16)$$

If we write

$$\underline{r}_C = \underline{r}_D + \underline{r}_{CD} \quad ,$$

we can perform the spatial integration as

$$\langle 1s(\underline{A}) | \cos(\underline{k}\cdot\underline{r}_C) | 1s(\underline{B}) \rangle = e^{-\left(\frac{\alpha_1 \alpha_2 r_{AB}^2}{\alpha_1 + \alpha_2}\right)} \Big\{ \cos(\underline{k}\cdot\underline{r}_{CD})$$

$$\times \int e^{-(\alpha_1 + \alpha_2) r_D^2} \cos(\underline{k}\cdot\underline{r}_D) \, d\tau$$

$$- \sin(\underline{k}\cdot\underline{r}_{CD}) \int e^{-(\alpha_1 + \alpha_2) r_D^2} \sin(\underline{k}\cdot\underline{r}_D) \, d\tau \Big\}$$

$$= \left[\frac{\pi}{\alpha_1 + \alpha_2}\right]^{3/2} e^{-\left(\frac{\alpha_1 \alpha_2}{\alpha_1 + \alpha_2}\right) r_{AB}^2} \cos(\underline{k}\cdot\underline{r}_{CD}) \, e^{-\left[\frac{k^2}{4(\alpha_1 + \alpha_2)}\right]} . \quad (2.17)$$

This is the expression for the s-s integral given in Appendix A. Expressions for other symmetry pairs are given in Appendix A along with expressions for the kinetic energy integrals given by eq. (2.5).

The use of GTO's is open to the criticism that the representation of an atomic wave function in terms of such orbitals is more cumbersome than with Slater type orbitals (STO). More GTO's than STO's must be included to obtain a similar degree of accuracy. This criticism is justified, but it is outweighed by the superior ease of calculation with GTO's. Analytic expressions for the S_{jn} are not known on an STO basis; instead a rather intricate numerical integration must be performed. This work was first undertakened using STO's. However, the summation of the Fourier coefficients of the potential could only be carried out to approximately 28 rotationally independent reciprocal lattice vectors in a reasonable amount of computer time. It will be shown later how incorrect this was. On this basis, an accurate tight binding calculation for a crystal composed of atoms with as many electrons as nickel is not practical with a basis set of STO's.

The following specific set of basis functions were used in this calculation. Wave functions for all atomic states except 3d (1s, 2s, 3s, 4s, 2p, 3p, and 4p) were represented by the linear combinations of Gaussian orbitals determined from a free atom self consistent field calculation by Wachters (1970). Inclusion of core wave functions is necessary (just as in the OPW method) in order to avoid convergence difficulties associated with the lack of orthogonality of wave functions on different atoms. The accuracy of the representation of the 4s and 4p states in terms of atomic functions is perhaps questionable; however work by Lafon and Lin (1966) and Chaney et al (1970) show that excellent results can be obtained for s and p bands in alkali metals by this procedure.

On the other hand, we have seen some evidence in a preliminary calculation (Callaway et al, 1971) that the d electron wave functions in a solid may be appreciably different from those existing in the free atom. In order to allow for this possibility we used a set of five separate radial GTO's in the construction of the $\phi_j(k,r)$.

One can think of this as constructing the basis set with five different 3d one-electron wave functions, each consisting of a single GTO. Since the d state has five different angular types, this contributes twenty-five functions to our basis set. The orbital exponents used in defining these functions were the same as used by Wachters (1970).

With this choice of basis functions, we obtain a 38 x 38 matrix problem at a general point of the Brillouin zone. The d-d portion is 25 x 25, s-s is 4 x 4, and p-p is 9 x 9. With matrices of this size, it is possible to obtain energy levels at a reasonably large number of general points in the Brillouin zone.

The computation of the matrix elements H_{ij} involves a double summation over both the direct lattice and reciprocal lattice vectors, and convergence must be achieved in both. The degree of difficulty depends on the orbitals involved. Terms of s-s and s-p types present the greatest difficulty. Near a nucleus, s like wave functions are sharply peaked and p like functions have a large gradient. As a result, the summation over reciprocal lattice vectors require many terms. For example, approximately 8100 rotationally independent lattice vectors were included in sums for the s-s elements for the first five neighbors. As the results were still not entirely converged, the remainder of the sum was replaced by an integral, which was evaluated using

Filon's rule. Figure 1 shows the convergence for the first neighbor 4s-3s integral. The results of summing N terms and the values obtained by graphical extrapolation and by integrating the Fourier series are shown. Much more rapid convergence was obtained for elements involving d functions.

The 4s and 4p wave functions are highly extended in space. It was necessary to include forty shells of neighbors (rotationally independent vectors R_{μ}) in order to obtain convergence. There is, unfortunately, substantial cancellation in the computation of certain matrix elements. The d-d matrix elements converged much more rapidly. Only five shells of neighbors were required in this case. Figure 2 shows the R convergence of certain matrix elements.

A straight forward calculation of H yields some elements which are imaginary. The matrix described earlier is labeled as follows

	d	s	p
d			
s			
p			

.

This matrix is Hermitian, that is,

$$H_{ij}^{*} = H_{ji} \quad . \qquad (2.18)$$

For tight binding matrix elements, we have

$$H_{ij} = \sum_{\mu} e^{i\underline{k}\cdot\underline{R}_{\mu}} E_{ij}(\underline{R}) \tag{2.18}$$

so that

$$H_{ij}^{*} = \sum_{\mu} e^{-i\underline{k}\cdot\underline{R}_{\mu}} E_{ij}^{*}(\underline{R}) = H_{ji} \quad . \tag{2.19}$$

But, the $E_{ij}(R)$ are all real quantities, and for a cubic crystal with inversion symmetry we have that for each $\underline{R}$ there exist a vector $-\underline{R}$. Sums over $\underline{R}$ are identical to sums over $-\underline{R}$. Now $E_{ij}(\underline{R})=-E_{ij}(-\underline{R})$ if i and j have different parity (s-p or p-d), but $E_{ij}(\underline{R})=E_{ij}(-\underline{R})$ if i and j have the same parity (s-s, p-p, d-d, and s-d). Thus, eq. (2.19) can be written

$$H_{ij}^{*} = H_{ji} = (-1)^{l_i + l_j} H_{ij} \tag{2.20}$$

where l_i=1,2,3(s,p,d). Thus, for i and j of different parity, $H_{ij}=-H_{ij}$, which means that H_{ij} is pure imaginary.

We label the matrix elements as follows, indicating explicity the imaginary factors

$$H_{ij} = \begin{pmatrix} H_{dd} & H_{sd} & iH_{dp} \\ H_{sd} & H_{ss} & iH_{sp} \\ -iH_{dp} & -iH_{sp} & H_{pp} \end{pmatrix} \quad . \tag{2.21}$$

We can make a unitary transformation, $H' = \mathcal{U} H \mathcal{U}^{-1}$, where

$$\mathcal{U} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & i \end{pmatrix} \quad \text{and} \quad \mathcal{U}^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -i \end{pmatrix} \qquad (2.22)$$

which gives

$$H'_{ij} = \begin{pmatrix} H_{dd} & H_{sd} & H_{dp} \\ H_{sd} & H_{ss} & H_{sp} \\ H_{dp} & H_{sp} & H_{pp} \end{pmatrix} . \qquad (2.23)$$

Here H'_{ij} is explicitly real and symmetric but the d-p and s-p blocks must be calculated with care to avoid an error of a negative sign on one of the blocks. Since the expression given is for $\langle P(\underline{A})/\hat{\mathcal{O}}/\ S(\underline{B})\rangle$, one can extact $\langle S(\underline{A})/\hat{\mathcal{O}}/\ P(\underline{B})\rangle$ simply by negation or by interchanging the values of $\underline{A}$ and $\underline{B}$ in the first equation from that used in the evaluation of the other expressions. Thus, H'_{ij} is the Hamiltonian matrix which appears in the secular eq. (2.2).

CHAPTER III

The Crystal Potential

The crystal potential was constructed as follows: It was assumed that the charge density of electrons in the crystal could be represented as a superposition of partially overlapping charge densities for individual nickel atoms in a $3d^9 4s^1$ configuration. The individual atomic charge densities were chosen to be spherically symmetric; however, the superposed density has only cubic symmetry about any lattice site. The wave functions used in forming the charge density were taken from the Hartree-Fock self consistent field calculation of Clementi (1965) for the free nickel atom in the $3d^8 4s^2 (^3F)$ configuration. These wave functions were linear combinations of Slater type Orbitals, which are given by Clementi (1965).

For reasons already discussed, we are interested in expanding this crystal potential in a Fourier series. The Fourier coefficients are given by

$$V(\underline{K}) = \frac{1}{N\Omega_0} \int V(\underline{r})\, e^{-i\underline{K}\cdot\underline{r}}\, d^3r$$

$$= \frac{1}{N\Omega_0} \left[\sum_{\mu} \int e^{-i\underline{K}\cdot\underline{r}}\, V_A(\underline{r}-\underline{R}_\mu)\, d^3r \right. \qquad (3.1)$$

where Ω_0 is the unit cell volume and N is the number of unit cells. Now, make a change of variables from

$\underline{r}$ to $\underline{r} + \underline{R}_\mu$, and we have

$$V(\underline{K}) = \frac{1}{N\Omega_o} \sum_\mu e^{-i\underline{K}\cdot\underline{R}_\mu} \left[\int V_A(\underline{r})\, e^{-i\underline{K}\cdot\underline{r}}\, d^3r \right]. \quad (3.2)$$

One makes use of the fact that

$$\sum_\mu e^{-i\underline{K}\cdot\underline{R}_\mu} = N \sum_K \delta_{\underline{K},\underline{K}_n} \quad (3.3)$$

where $\underline{K}_n$ is a reciprocal lattice vector, and we have

$$V(\underline{K}_n) = \frac{1}{\Omega_o} \int V_A(r)\, e^{-i\underline{K}_n\cdot\underline{r}}\, d^3r \; . \quad (3.4)$$

Each of the atomic potentials has the form

$$V(\underline{r}_2) = -\frac{2Z}{r_2} + 2\int \frac{\rho(r_1)}{r_{12}}\, d^3r_1 \quad (3.5)$$

where Z is the atomic number and $\rho(r)$ is the electron charge density. The factors of 2 converts the energy into Rydbergs (atomic units with energies in rydbergs are used throughout this paper). The charge density is given by

$$\begin{aligned} \rho(r) &= \sum_i a_i |\psi_i|^2 \\ &= 2|\psi_{1s}|^2 + 2|\psi_{2s}|^2 + 6|\psi_{2p}|^2 + 2|\psi_{3s}|^2 \\ &\quad + 6|\psi_{3p}|^2 + 9|\psi_{3d}|^2 + |\psi_{4s}|^2 \end{aligned} \quad (3.6)$$

where the a_i is the occupation number of the i-th state. Thus, the Fourier coefficients are given as

$$V(\underline{K}) = \frac{-2Z}{\Omega_o}\int \frac{e^{i\underline{K}\cdot\underline{r}_2}}{r_2} d^3r + \frac{2}{\Omega_o}\iint \frac{\rho(\underline{r}_1)}{|\underline{r}_{12}|} e^{-i\underline{K}\cdot\underline{r}_2} d^3r_1 d^3r_2 . \quad (3.7)$$

Using the identity

$$\int \frac{e^{-i\underline{K}\cdot\underline{r}_2}}{|\underline{r}_{12}|} d^3r_2 = \frac{4\pi}{K^2} e^{-i\underline{K}\cdot\underline{r}_1} \quad (3.8)$$

and performing the simple integrals remaining, we obtain the final result

$$V(\underline{K}) = \frac{-8\pi Z}{\Omega_o K^2} + \frac{32\pi^2}{\Omega_o K^3}\int_0^\infty \rho(\underline{r}_1)\, r_1 \sin(Kr_1)\, dr_1 \quad . \quad (3.9)$$

Now the charge density is spherially averaged as

$$\rho(\underline{r}) = \frac{1}{4\pi}\sum_i a_i |u_i|^2 \quad (3.10)$$

where u_i is the radial part of the wave function, that is, replace ψ_i by $u_i \times Y_{oo}(\theta,\phi)$ in (3.6).

The expression (3.9) is not valid for $\underline{K}$=0. However, expanding the sine term and taking the limit $V(\underline{K})$ as $\underline{K}\to 0$, we have

$$V(0) = \lim_{K\to 0}\left[\frac{-8Z}{K^2} + \frac{8\pi}{K^3}\int \sum_i a_i |u_i(\underline{r}_1)|^2 \left[Kr_1 - \frac{(Kr_1)^3}{3!} + \cdots\right] r_1 dr_1\right.$$

$$= \frac{-8Z}{\Omega_o K^2} + \frac{8Z}{\Omega_o K^2} - \frac{4\pi}{3\Omega_o}\int_0^\infty \sum_i a_i |u_i(\underline{r}_1)|^2 r_1^4 dr_1$$

$$= \frac{-4\pi}{3\Omega_0}\int_0^{\infty}\sum_i a_i |u_i(\underline{r}_1)|^2 r_1^4\, dr_1 \quad . \tag{3.11}$$

These expressions can be readily evaluated analytically.

The validity of our approximation in the formulation of the Coulomb and exchange potentials used in the Hamiltonian above was first shown by Slater (1951). The Hartree-Fock equations (Slater , 1930) furnish the best set of one-electron wave functions for use in describing the motion of electrons in the field of atomic nuclei. However, they are so complicated to use, specifically the exchange term, that they have not been employed except in relatively simple cases. The Hartree-Fock equations can be written in the form

$$H_1 u_i(\underline{x}_1) + \left[\sum_{k=1}^{n}\int u_k^*(\underline{x}_2)\, u_k(\underline{x}_2)\frac{e^2}{|\underline{r}_{12}|}\, dx_2\right] u_i(\underline{x}_1)$$

$$-\sum_{k=1}^{n}\left[\int u_k^*(\underline{x}_2)\, u_i(\underline{x}_2)\frac{e^2}{|\underline{r}_{12}|}\, dx_2\right] u_k(\underline{x}_1) = E_i\, u_i(\underline{x}_1) \tag{3.12}$$

where H_1 is the kinetic energy operator, $u_i(\underline{x})$ are the one-electron wave functions, and n is the number of one-electron states associated with the atom. The second term is the Coulomb potential energy and the third term is the exchange potential energy. Taking the summation in the Coulomb term inside the integral, we have the charge density as given in eq. (3.6). However, the exchange term cannot be computed as shown; therefore, we make use of the Hartree-Fock-Slater approximation (Slater, 1951) described below.

A local exchange potential for an electon of spin σ was constructed using the "$X\alpha$" method of Slater et al (1969) which is

$$V_{ex,\sigma}(\underline{r}) = -6\alpha\left[\frac{3\rho_\sigma(\underline{r})}{4\pi}\right]^{1/3} \tag{3.13}$$

where α is an empirical constant ranging from 2/3 to 1.

In this expression ρ_σ is the total charge density of electrons of spin σ. This charge density was constructed by adding the overlapping distributions produced by neutral atoms in the configuration mentioned above placed on the face center cubic lattice sites. Again, we are interested in obtaining the Fourier coefficients of the exchange potential, which are given by

$$V_{ex,\sigma}(\underline{K}) = \frac{\alpha}{\Omega_0}\frac{4\pi}{K_s}\int -6\left(\frac{3\rho_\sigma(\underline{r})}{4\pi}\right)^{1/3} \sin(K_s r)\, r\, dr \,. \tag{3.14}$$

The charge density $\rho_\sigma(\underline{r})$ is given just as (3.10), that is,

$$\rho_\sigma(\underline{r}) = \frac{1}{4\pi}\sum_i a_{i\sigma}|u_i|^2 \tag{3.15}$$

where the $a_{i\sigma}$'s now depend on the spin orientation. The charge density for the crystal was found at selected points within spheres centered about each nickel atom and having radii equal to half the nearest neighbor distance. These points were chosen to be values of r ranging from 0 to the radius of the sphere. Then, using this numerical charge density, a 96 point Gaussian formula for numerical integration was used to calculate all the Fourier coefficients $V_{ex,\sigma}(\underline{K}_s)$ (Norwood, 1970). The charge density was found by summing contributions from atomic charge densities out through nine sets of neighbors.

The Slater approximation for an effective exchange potential can be used to investigate the band structure of a ferromagnetic metal. The exchange potential for an electron of given spin is determined by the electron distribution for the spin. When the numbers of electrons in states of up and down spin are different, the exchange potential will tend to cause a splitting of the band structure. This approach was first applied in a study of energy bands in ferromagnetic iron by Callaway (1955), and has subsequently been employed by Wakoh (1965) and Connolly (1967) in studies of nickel.

Dannan et al (1968) have measured the magneton number (the difference in the number of electrons occupying the up spin and down spin states) to be 0.56 electrons per atom, and due to d electrons only. In order to use the same basis set of functions in the secular equation, we need Fourier coefficients of the exchange potential calculated from a common set of wave functions for both up and down spins. This is accomplished by fixing the occupation of each electron state in the $3d^9 4s^1$

configuration and calculating a spin dependent charge density. Thus, we have artificially introduced a spin dependent exchange potential to effect a spin splitting. Specifically, the occupation numbers appearing in (3.10) were

	1s	2s	3s	4s	2p	3p	3d
up spin $a_{i\sigma}$	1	1	1	.5	3	3	4.78
down spin $a_{i\sigma}$	1	1	1	.5	3	3	4.22

The original Slater exchange potential (1951) has $\alpha = 1$; the Kohn-Sham-Gasper potential (1965) has $\alpha = 2/3$. In the present calculation, we investigated the effects of the variation of α between these limits. The results appeared to be more satisfactory when α was close to unity. The parameter α was chosen in the following way: It was observed that the relative position of the p and d like levels at the Brillouin zone point L was quite sensitive to the value of α. This occurs because the d band level L_3 varies considerably more rapidly with α than p like state L_2'. There is experimental evidence indicating that $L_2'(\uparrow)$ should be about 0.4 ev below the Fermi energy. This is achieved for $\alpha \simeq 0.972$, which was the value adopted.

This procedure has been criticized by Herring (1966) and others who argue that an electron in a ferromagnetic metal cannot be regarded as experiencing an average exchange potential originating from atoms, all of which are in the same average configuration. Alternate procedures based on an approximate treatment of electron correlation in narrow bands have been employed (Hodges et al, 1966; Callaway and Zhang, 1970). In view of the criticisms of Slater's procedure, it may be surprising that the results, at least in the case of nickel, are in fair agreement with other approaches by Hodges et al (1966) and Callaway and Zhang (1970) and with experiment. For example, Connolly (1967) obtains a magneton number of 0.62 (in comparison with the experimental value of 0.56). Our result of 0.69 is not greatly different.

CHAPTER IV

Self Consistency

For some time, the tight binding method has been regarded as suitable only for a simple first approximation to a complex band structure. However, Lin and Lafon (1966) have shown that the method is quite powerful in quantitative calculations from first principles. In this chapter, we will describe a procedure by which self consistent band calculations may be performed using the tight binding method. The practicality of this technique is seen in the fact that iterated Fourier coefficients of the potential can be obtained from the matrix elements of the Hamiltonian. Thus, for a fixed set of basis functions, these integrals need only be computed once. A printout of the computer program which performs this self consistent calculation is listed in Appendix B.

The fundamental problem is to determine an iterated potential after a given band structure calculation has been completed. Hence, one has a definite set of energy bands $E_n(\underline{k})$ and Bloch functions $\psi_n(\underline{k},\underline{r})$ which have been obtained by diagonalization of the Hamiltonian and overlap matrices resulting from some assumed set of wave functions. The Bloch functions are

$$\psi_n(\underline{k},\underline{r}) = \sum_i a_{ni}(\underline{k})\, \phi_i(\underline{k},\underline{r}) \tag{4.1}$$

where the $a_{ni}(\underline{k})$ are the eigenvectors of the diagonalization process and the $\phi_i(\underline{k},\underline{r})$ are the tight binding functions for wave vector $\underline{k}$:

$$\phi_i(\underline{k},\underline{r}) = \frac{1}{\sqrt{N}}\sum_{\mu} e^{i\underline{k}\cdot\underline{R}_\mu} u_i(\underline{r}-\underline{R}_\mu) \qquad (4.2)$$

where the summation runs over all N lattice sites, R_μ.

Since all that is required in the method used are the Fourier coefficients of the potential, the iterated values of $V(\underline{K})$ are all that is needed. For $K \neq 0$, the coefficients of the Coulomb potential are related to the charge density by (Callaway, 1964)

$$V(\underline{K}) = -8\pi \frac{\rho(\underline{K})}{K^2} \qquad (4.3)$$

(in atomic units, with energies in Rydbergs). The Fourier coefficients of $\rho(\underline{K})$ are given by

$$\rho(\underline{K}) = \frac{1}{N\Omega_0}\int \rho(\underline{r})\, e^{-i\underline{K}\cdot\underline{r}}\, d^3r \qquad (4.4)$$

where Ω_0 is the volume of the unit cell and

$$\rho(\underline{r}) = \sum_{n,\underline{k}} |\psi_n(\underline{k},\underline{r})|^2 \qquad (4.5)$$

with the summation over only occupied states. Substituting and converting the sum on $\underline{k}$ to an integral, we have

$$\rho(\underline{K}) = \frac{1}{(2\pi)^3}\sum_{n,i,j}\int d^3k\, a^*_{ni}(\underline{k})\, S_{ij}(\underline{k},\underline{K})\, a_{nj}(\underline{k}) \qquad (4.6)$$

where the integral is over only that portion of the Brillouin zone in which band n is occupied. The quantities S_{ij} are generalized overlap matrix elements

$$S_{ij}(\underline{k},\underline{K}) = \sum_{\sigma} e^{i\underline{k}\cdot\underline{R}_\sigma} \int u_i^*(\underline{r}) e^{-i\underline{K}\cdot\underline{r}} u_j(\underline{r}-\underline{R}_\sigma)\, d^3r \,. \quad (4.7)$$

The integrals appearing in (4.7) are exactly those which are required in the computation of the matrix elements of the Hamiltonian on the basis of the functions $\phi_i(\underline{k},\underline{r})$. Specifically, we have

$$\int \phi_i^*(\underline{k},\underline{r})\, V(\underline{r})\, \phi_j(\underline{k},r)\, d^3r$$

$$= \sum_{s,\sigma} V(\underline{K}_s)\, e^{i\underline{k}\cdot\underline{R}_\sigma} \int u_i(\underline{r}) e^{i\underline{K}_s\cdot\underline{r}} u_j(\underline{r}-\underline{R}_\sigma)\, d^3r$$

$$= \sum_{s} V(\underline{K}_s)\, S_{ij}(\underline{k},-\underline{K}_s) \quad (4.8)$$

in which $V(\underline{r})$ is the periodic crystal potential. If a fixed set of basis functions is employed, the quantities S_{ij} need be computed only once.

To simplify these computations, we can write

$$H_{ij}(\underline{k}) = H_{ij}^{\circ}(\underline{k}) + \sum_{K}\left(\Delta V_c(\underline{k}) + \Delta V_{ex}(\underline{k})\right) S_{ij}(\underline{k},\underline{K}) \quad (4.9)$$

where the Δ implies the change in the Fourier coefficients from one iteration to the next. With this, we need matrices of the type

$$O_{ij} = \sum_{\sigma} e^{i\underline{k}\cdot\underline{R}_\sigma} \int u_i^*(\underline{r})\, O\, u_j(\underline{r}-\underline{R}_\sigma)\, d^3r \quad (4.10)$$

where O is one of the quantities; kinetic energy, overlap, potential, or r^2. Hence, $H_{ij}^{\circ}(\underline{k})$ is merely the sum of the kinetic, Coulomb potential, and exchange potential energies.

In the case of K = 0, the Fourier coefficient of the Coulomb potential is determined by a limiting process

$$V(0) = -8\pi \lim_{K\to 0} \frac{\rho(\underline{K})}{K^2} . \tag{4.11}$$

The limit exists, and is expressed as

$$V(0) = \frac{1}{6\pi^2} \sum_{n,i,j} \int a^*_{n_i}(\underline{k})\, S^{(2)}_{ij}(\underline{k})\, a_{n_j}(\underline{k})\, d^3 r \tag{4.12}$$

where

$$S^{(2)}_{ij}(\underline{k}) = \sum_{\sigma} e^{-i\underline{k}\cdot\underline{R}_\sigma} \int u_i^*(\underline{r})\, r^2\, u_j(\underline{r}-\underline{R}_\sigma)\, d^3 r . \tag{4.13}$$

In the Slater "Xα" approach, the exchange potential is then proportional to $\rho^{1/3}(\underline{r})$. If one assumes that the changes in the Fourier coefficients are small in subsequent steps, we can proceed as follows: Let $\rho^{1/3}(\underline{r})$ be the cube root of the charge density at the present stage of iteration, and let $\rho_o^{1/3}(\underline{r})$ be the same quantity at the preceeding stage. We write

$$\rho^{1/3}(\underline{r}) = \rho_o^{1/3}(\underline{r}) + \Delta(\underline{r}) . \tag{4.14}$$

$\Delta(\underline{r})$ is expanded in a Fourier series,

$$\Delta(\underline{r}) = \sum_{s} \Delta(\underline{K}_s)\, e^{-i\underline{K}_s\cdot\underline{r}} \tag{4.15}$$

from which we obtain the Fourier transform of the change in charge density, $\Delta(\underline{K}_s)$ by expansion

$$\Delta(\underline{K}) = \frac{1}{3}\left(\frac{\Omega_o}{n_e}\right)^{2/3} \Big\{ \rho(\underline{K}) - \rho_o(\underline{K}) - \frac{2}{3}\left(\frac{\Omega_o}{n_e}\right) \sum_{\tau\neq 0} \rho(\underline{K}_\tau)\rho(\underline{K}-\underline{K}_\tau) - \rho_o(\underline{K}_\tau)\rho_o(\underline{K}-\underline{K}_\tau) \Big\} \tag{4.16}$$

where only second order terms have been retained. The quantity n_e is the number of electrons in the cell.

In the case K = 0, we use a consequence of the use of normalized Bloch functions that

$$\rho(0) = \frac{n_e}{\Omega_0} \tag{4.17}$$

at each stage of the iteration. Consequently,

$$\Delta(0) = -\frac{2}{9}\left(\frac{\Omega_0}{n_e}\right)^{5/3}\sum_{\tau}\left[\rho(\underline{K}_\tau)\rho(-\underline{K}_\tau) - \rho_0(\underline{K}_\tau)\rho_0(-\underline{K}_\tau)\right] \tag{4.18}$$

The use of these approximate formulas $\Delta(\underline{K})$ is dependent on the assumption that the changes in the Fourier coefficients of ρ are small.

CHAPTER V

Results

Energy levels for both the up and down spins were obtained at 1505 independent points in 1/48'th of the Brillouin zone. The points chosen may be characterized by integer values, (n_x, n_y, n_z), representing the coordinate $(K_x, K_y, K_z) = \frac{2\pi}{24a}(n_x, n_y, n_z)$ such that $n_x \geq n_y \geq n_z$ and the symmetry point X has the coordinate $\frac{2\pi}{24a}(24, 0, 0)$, where a is the lattice constant. Also, we have the restriction that $(n_x+n_y+n_z) \leq 36$ such that the coordinates remain in the 1/48'th partition of interest. Portions of the band structures along certain symmetry directions for majority (up) and minority (down) spins are shown in figure (3) and (4) respectively. The results are qualitatively similar to those obtained by Connolly (1967) and others. The band structure shows the characteristic interlacing d bands, partially hybridized with an overlapping broad band. A p state, L_2', enters the d band region at the center of a hexagonal zone face.

Certain characteristic energy differences between states are listed in Table III. The X_5-X_1 separation is a rough measure of the d band width, while Γ_1-X_4' gives the width of the overlapping s-p band. We obtain a d band width of 0.324 ry for both spins while Connolly (1967) obtains 0.33 ry for up spin and 0.36 ry for down spin and Zornberg (1970) obtains a separation of approximately 0.38 ry. Comparison of the s-p band width shows Connolly (1967) with a separation of 0.84 ry, Zornberg with a separation of approximately 0.87 ry, and our work with a separation of 0.81 ry for each spin. Hence these theoretical calculations agree moderately well, especially when one considers that each was done by a different method using different crystal potentials.

A significant feature of the band structure of nickel is the very flat highest d band, connecting the states X_5 and W_1'. If only nearest neighbor interactions were considered, this band would be absolutely flat. Second neighbor and higher order interactions produce a slight deviation of the energy of this band from constancy, but this is quite small: the energy variation between these states is only 4×10^{-5} ry.

Some values for the energy differences between states of up and down spin are specified in Table IV. It can be seen from this table that while the splitting of d like states is not constant, it does not vary very much, remaining in the neighborhood of 0.06 ry or 0.8 ev. On the other hand, the splitting of predominately s and p like states tends to be smaller by a factor of approximately three. The present results for the spin splitting of d like states are in reasonable agreement with those obtained in a previous calculation using t matrix techniques (Callaway and Zhang, 1970), and also with those obtained by others using the Slater procedure such as Wakoh (1965) and Connolly (1967). Our result is, however, larger by a factor of approximately two than values considered by Zornberg (1970) as giving reasonable agreement with optical measurements. Specifically, we obtain spin splitting of 0.06 ry for $\Delta\Gamma_{25'}$ and 0.022 ry for $\Delta\Gamma_1$. Connolly has $\Delta\Gamma_{25'} = 0.07$ ry and $\Delta\Gamma_1 = 0.016$ ry.

Experimental results are available from some optical measurements such as those by Stoll (1970) and Krinchik et al (1968). Stoll (1970) suggests that the X_5 level must be situated approximately 0.22 ry above the Fermi level. We have X_5 at 0.27 ry above the Fermi energy, indicating that our Fermi energy is well situated with respect to the s-p bands. He further indicates that the d band spin splitting ($\Delta\Gamma_{25'}$) should be of the order of 0.026 ry, hence the factor of two mentioned earlier. However, our splitting of the p level X_4' is three times larger than Stoll's (1970) values of 0.008 ry. Krinchik et al (1968) agree with our relative position of L_2', that is, L_2' below L_{32} for the down spin with the Fermi energy between them, and L_2' above L_{32} in the up spin with the Fermi energy above L_2'. However, they indicate that $L_2'(\uparrow) - L_2'(\downarrow)$ should be approximately 0.005 ry; whereas, we obtained 0.002 ry. They also obtained $L_{32}(\uparrow) - L_{32}(\downarrow) = 0.032$ ry in comparison to 0.065 ry in our calculation. This data further substantiates the fact that this calculation has the spin splitting too large by approximately a factor of two.

A rough density of states was obtained by simple state counting techniques. The subroutine which calculates the density of states is included in the band program listed in Appendix B. Results for majority, minority, and total densities are presented in figures (5), (6), and (7). The densities are nearly the same except for a shift in energy corresponding to the spin splitting.

The Fermi energy was determined from the density of states and was found to be approximately -0.493 ry for the $\alpha \simeq 0.972$ used in this calculation. The magneton number, which is the difference between the number of occupied states of majority spin, and the number of occupied minority spin states, was found to be 0.69. This is somewhat larger than the experimental value of 0.56 given by Dannan et al (1968). The total density of states at the Fermi energy is 24 electron states/atom-ry.

Determination of the Fermi energy makes possible the investigation of the Fermi surface. Certain cross sections of the predicted Fermi surface are shown in figures (8) and (9) which refer to majority and minority spins, respectively, Some properties of the Fermi surface are listed in Table V.

The majority spin portion of the Fermi surface lies entirely in the upper (s-p) band 6. Qualitatively, it is similar to the Fermi surface of copper: a distorted sphere with necks making contact with the Brillouin zone boundary around L. The neck areas given in the table are somewhat larger than implied by the experimental results of Tsui (1967). For example, we obtained 0.0093 a. u. compared to 0.0072 a. u. from Tsui (1967). It is probable that the L_2' level has been placed slightly too far below the Fermi energy.

The minority spin portion of the Fermi surface is considerably more complicated. In the first place, we find the hole pockets at X which have been observed in the de-Haas van Alphen effect measurements. Our results for the size of this pocket, which is associated with the X_5 level, are in rather good agreement with the experimental measurements. This calculation found a second pocket of minority spin holes (3d band) near X, associated with the X_2 level. Such holes have not been observed experimentally, although they have been predicted by other first principle calculations as well (Connolly, 1967). If there are, in fact, no such holes, the discrepancy in this calculation could be explained by a slightly too low placement of the Fermi level; the actual position of the Fermi level would then come between X_5 and X_2.

There are large portions of the minority spin Fermi surface which have not yet been observed: that associated with band 5 holes presumably responsible for the ferromagnetism and the band 6 electrons. Measurement of the properties of these portions of the Fermi surface would be of considerable importance in testing band calculations.

For general interest, we present here numerical values for integrals of importance for conventional tight binding calculations for d bands. These quantities are the matrix elements $S_{ij}(\underline{K},\underline{R})$ discussed in Chapter II, in which i and j denote d states, given for central cell, first, and second neighbors (R = (0,0,0), a/2(1,1,0), and a/2(0,0,2)). These values are given in Table II for the sum of kinetic energy and ordinary (Coulomb) potential energy, the exchange energy (full Slater for the paramagnetic state), and overlap integrals. These integrals were determined using the d-d integral computer program listed in Appendix B with the d state atomic wave functions of Wachters (1970). In the calculations described in the main text of this paper, we used Bloch functions formed from individual Gaussian orbitals rather than complete atomic wave functions; however, integrals based on atomic wave functions are interesting for purposes of comparison with values obtained by various interpolation schemes.

Many authors have considered the so-called two center approximation (Slater and Koster, 1954), in which three center integrals occurring in the usual form of the tight finding method are neglected. There are several different combinations of the integrals E_{ij} which can be used to determine values of the independent d type two center integrals, denoted as (ddσ), (ddπ), and (ddδ).

In fact, Slater and Koster (1954) list the integrals E_{ij} in terms of the two center integrals. These results would agree exactly if the two center approximations were accurate. These expressions can be solved to give the two center integrals in terms of E_{ij}. There are eight independent expressions for $(dd\pi)$, six independent expressions for $(dd\delta)$, and twelve independent expressions for $(dd\sigma)$. An example of each is

$$(dd\pi) = E_{xy,xy}(101) + E_{xy,xz}(011)$$

$$(dd\sigma) = \frac{3}{2} E_{xy,xy}(110) - \frac{1}{2} E_{3z^2-r^2,3z^2-r^2}(110)$$

$$(dd\delta) = E_{xy,xy}(110) + \sqrt{3}\, E_{xy,3z^2-r^2}(110)$$

Numerical values for these two center integrals are compared in Table VI with those obtained by other authors. Only mean values for the nearest neighbor two center parameters obtained from Table II are presented. The spread is not large except in the case of the integral of smallest magnitude, $(dd\delta)$. There is some measure of agreement with the values obtained by fits to APW calculations. The discrepancies with the values of Fletcher and Wohlfarth (1951) would be substantially reduced if the contribution from the exchange potential to our values was deleted, since they did not include exchange in their calculations.

As a closing note, the self consistency procedure described in Chapter IV will be discussed briefly. A computer program, which is listed in Appendix B, has been written to perform this calculation. However, final results have not been obtained at this time, but should be available in the near future. This work is to be continued by members of the Solid State Physics group at Louisiana State University. Enough work has been done thus far to clearly indicate that the spin splitting will decrease with self consistency.

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TABLE I

IN THIS TABLE, THE FOURIER COEFFICIENTS OF THE COULOMB, PARAMAGNETIC EXCHANGE, UP-SPIN EXCHANGE, AND DOWN-SPIN EXCHANGE POTENTIALS ARE PRESENTED. ONLY THE FIRST 100 UNIQUE SHELLS ARE SHOWN SINCE 8184 WERE ACTUALLY USED AND CANNOT BE PRESENTED HERE.

KX	KY	KZ	COULOMB	PARAMAGNETIC	UP-SPIN	DOWN-SPIN
0	0	0	-0.160747E 01	-0.130430E 01	-0.131756E 01	-0.129074E 01
1	1	1	-0.873536E 00	-0.273472E 00	-0.276379E 00	-0.270497E 00
2	0	0	-0.787361E 00	-0.150984E 00	-0.152479E 00	-0.149455E 00
2	2	0	-0.583833E 00	-0.415256E-01	-0.413557E-01	-0.417091E-01
3	1	1	-0.493872E 00	-0.576511E-01	-0.575919E-01	-0.577223E-01
2	2	2	-0.469955E 00	-0.598546E-01	-0.598548E-01	-0.598643E-01
4	0	0	-0.393727E 00	-0.440740E-01	-0.441719E-01	-0.439786E-01
3	3	1	-0.350809E 00	-0.210042E-01	-0.210504E-01	-0.209576E-01
4	2	0	-0.338451E 00	-0.140305E-01	-0.140511E-01	-0.140091E-01

TABLE I (CONTINUED)

4	2	2	-0.296406E 00	0.323680E-02	0.329997E-02	0.317480E-02
5	1	1	-0.270933E 00	0.449103E-02	0.457269E-02	0.441029E-02
3	3	3	-0.270933E 00	0.449103E-02	0.457269E-02	0.441029E-02
4	4	0	-0.236721E 00	-0.553755E-02	-0.549152E-02	-0.558315E-02
5	3	1	-0.219934E 00	-0.120664E-01	-0.120511E-01	-0.120815E-01
4	4	2	-0.214840E 00	-0.136827E-01	-0.136757E-01	-0.136897E-01
6	0	0	-0.214840E 00	-0.136827E-01	-0.136757E-01	-0.136897E-01
6	2	0	-0.196575E 00	-0.163211E-01	-0.163294E-01	-0.163131E-01
5	3	3	-0.184757E 00	-0.145423E-01	-0.145430E-01	-0.145423E-01
6	2	2	-0.181123E 00	-0.134229E-01	-0.134180E-01	-0.134283E-01
4	4	4	-0.167900E 00	-0.767398E-02	-0.763952E-02	-0.770957E-02
7	1	1	-0.159180E 00	-0.339408E-02	-0.333650E-02	-0.345307E-02
5	5	1	-0.159180E 00	-0.339408E-02	-0.333650E-02	-0.345307E-02
6	4	0	-0.156471E 00	-0.218545E-02	-0.212120E-02	-0.225118E-02
6	4	2	-0.146506E 00	0.954338E-03	0.103634E-02	0.870686E-03

TABLE I (CONTINUED)

7	3	1	-0.139837E 00	0.134884E-02	0.143327E-02	0.126277E-02
5	5	3	-0.139837E 00	0.134884E-02	0.143327E-02	0.126277E-02
8	0	0	-0.129999E 00	-0.104061E-02	-0.970101E-03	-0.111250E-02
7	3	3	-0.124750E 00	-0.347169E-02	-0.341599E-02	-0.352856E-02
6	4	4	-0.123097E 00	-0.432039E-02	-0.426999E-02	-0.437189E-02
8	2	0	-0.123097E 00	-0.432039E-02	-0.426999E-02	-0.437189E-02
8	2	2	-0.116913E 00	-0.740486E-02	-0.737451E-02	-0.743600E-02
6	6	0	-0.116913E 00	-0.740486E-02	-0.737451E-02	-0.743600E-02
7	5	1	-0.112684E 00	-0.900239E-02	-0.898354E-02	-0.902189E-02
5	5	5	-0.112684E 00	-0.900239E-02	-0.898354E-02	-0.902189E-02
6	6	2	-0.111344E 00	-0.935004E-02	-0.933402E-02	-0.936665E-02
8	4	0	-0.106304E 00	-0.974808E-02	-0.973786E-02	-0.975880E-02
9	1	1	-0.102828E 00	-0.907934E-02	-0.906788E-02	-0.909128E-02
7	5	3	-0.102828E 00	-0.907934E-02	-0.906788E-02	-0.909128E-02
8	4	2	-0.101723E 00	-0.870450E-02	-0.869172E-02	-0.871778E-02

TABLE I (CONTINUED)

6	6	4	-0.975401E-01	-0.668598E-02	-0.666467E-02	-0.670786E-02
9	3	1	-0.946351E-01	-0.490830E-02	-0.487875E-02	-0.493850E-02
8	4	4	-0.901821E-01	-0.219834E-02	-0.215593E-02	-0.224154E-02
9	3	3	-0.877186E-01	-0.104081E-02	-0.993109E-03	-0.108934E-02
7	7	1	-0.877186E-01	-0.104081E-02	-0.993109E-03	-0.108934E-02
7	5	5	-0.877186E-01	-0.104081E-02	-0.993109E-03	-0.108934E-02
8	6	0	-0.869291E-01	-0.760850E-03	-0.711971E-03	-0.810580E-03
10	0	0	-0.869291E-01	-0.760850E-03	-0.711971E-03	-0.810580E-03
10	2	0	-0.839179E-01	-0.213472E-03	-0.163104E-03	-0.264696E-03
8	6	2	-0.839179E-01	-0.213472E-03	-0.163104E-03	-0.264696E-03
9	5	1	-0.818021E-01	-0.382826E-03	-0.334692E-03	-0.431780E-03
7	7	3	-0.818021E-01	-0.382826E-03	-0.334692E-03	-0.431780E-03
6	6	6	-0.811221E-01	-0.536859E-03	-0.490045E-03	-0.584472E-03
10	2	2	-0.811221E-01	-0.536859E-03	-0.490045E-03	-0.584472E-03
9	5	3	-0.766822E-01	-0.253794E-02	-0.250603E-02	-0.257044E-02

TABLE I (CONTINUED)

10	4	0	-0.760901E-01	-0.289457E-02	-0.286525E-02	-0.292444E-02
8	6	4	-0.760901E-01	-0.289457E-02	-0.286525E-02	-0.292444E-02
10	4	2	-0.738171E-01	-0.429212E-02	-0.427314E-02	-0.431152E-02
11	1	1	-0.722060E-01	-0.518511E-02	-0.517308E-02	-0.519745E-02
7	7	5	-0.722060E-01	-0.518511E-02	-0.517308E-02	-0.519745E-02
8	8	0	-0.696824E-01	-0.611490E-02	-0.611135E-02	-0.611863E-02
11	3	1	-0.682572E-01	-0.626327E-02	-0.626242E-02	-0.626424E-02
9	7	1	-0.682572E-01	-0.626327E-02	-0.626242E-02	-0.626424E-02
9	5	5	-0.682572E-01	-0.626327E-02	-0.626242E-02	-0.626424E-02
10	4	4	-0.677959E-01	-0.624222E-02	-0.624187E-02	-0.624269E-02
8	8	2	-0.677959E-01	-0.624222E-02	-0.624187E-02	-0.624269E-02
8	6	6	-0.660161E-01	-0.583009E-02	-0.582970E-02	-0.583058E-02
10	6	0	-0.660161E-01	-0.583009E-02	-0.582970E-02	-0.583058E-02
11	3	3	-0.647456E-01	-0.522709E-02	-0.522485E-02	-0.522943E-02
9	7	3	-0.647456E-01	-0.522709E-02	-0.522485E-02	-0.522943E-02

TABLE I (CONTINUED)

10	6	2	-0.643337E-01	-0.498267E-02	-0.497954E-02	-0.498591E-02
8	8	4	-0.627407E-01	-0.386321E-02	-0.385554E-02	-0.387101E-02
12	0	0	-0.627407E-01	-0.386321E-02	-0.385554E-02	-0.387101E-02
11	5	1	-0.616004E-01	-0.295799E-02	-0.294639E-02	-0.296976E-02
7	7	7	-0.616004E-01	-0.295799E-02	-0.294639E-02	-0.296976E-02
12	2	0	-0.612301E-01	-0.265934E-02	-0.264641E-02	-0.267244E-02
12	2	2	-0.597952E-01	-0.155045E-02	-0.153261E-02	-0.156851E-02
10	6	4	-0.597952E-01	-0.155045E-02	-0.153261E-02	-0.156851E-02
11	5	3	-0.587653E-01	-0.870205E-03	-0.849443E-03	-0.891216E-03
9	7	5	-0.587653E-01	-0.870205E-03	-0.849443E-03	-0.891216E-03
12	4	0	-0.571302E-01	-0.146727E-03	-0.123311E-03	-0.170410E-03
9	9	1	-0.561948E-01	0.114995E-04	0.349677E-04	-0.122294E-04
8	8	6	-0.558902E-01	0.182656E-04	0.414898E-04	-0.521427E-05
10	8	0	-0.558902E-01	0.182656E-04	0.414898E-04	-0.521427E-05
12	4	2	-0.558902E-01	0.182656E-04	0.414898E-04	-0.521427E-05

TABLE I (CONTINUED)

10	8	2	-0.547061E-01	-0.166972E-03	-0.145947E-03	-0.188219E-03
9	9	3	-0.538523E-01	-0.497642E-03	-0.479384E-03	-0.516082E-03
11	5	5	-0.538523E-01	-0.497642E-03	-0.479384E-03	-0.516082E-03
11	7	1	-0.538523E-01	-0.497642E-03	-0.479384E-03	-0.516082E-03
13	1	1	-0.538523E-01	-0.497642E-03	-0.479384E-03	-0.516082E-03
10	6	6	-0.535739E-01	-0.636891E-03	-0.619728E-03	-0.654222E-03
12	4	4	-0.524902E-01	-0.129452E-02	-0.128235E-02	-0.130680E-02
13	3	1	-0.517073E-01	-0.184375E-02	-0.183567E-02	-0.185189E-02
11	7	3	-0.517073E-01	-0.184375E-02	-0.183567E-02	-0.185189E-02
9	7	7	-0.517073E-01	-0.184375E-02	-0.183567E-02	-0.185189E-02
10	8	4	-0.514518E-01	-0.202804E-02	-0.202133E-02	-0.203478E-02
12	6	0	-0.514518E-01	-0.202804E-02	-0.202133E-02	-0.203478E-02
12	6	2	-0.504557E-01	-0.272692E-02	-0.272551E-02	-0.272829E-02
13	3	3	-0.497349E-01	-0.317008E-02	-0.317219E-02	-0.316788E-02
9	9	5	-0.497349E-01	-0.317008E-02	-0.317219E-02	-0.316788E-02

TABLE I (CONTINUED

8	8	8	-0.485803E-01	-0.366436E-02	-0.367090E-02	-0.365766E-02
11	7	5	-0.479141E-01	-0.378455E-02	-0.379271E-02	-0.377621E-02
13	5	1	-0.479141E-01	-0.378455E-02	-0.379271E-02	-0.377621E-02
12	6	4	-0.476962E-01	-0.379345E-02	-0.380195E-02	-0.378475E-02
14	0	0	-0.476962E-01	-0.379345E-02	-0.380195E-02	-0.378475E-02

TABLE II

In this table we give some d-d matrix elements used in our calculation. They are given for the sum of the potential energy and kinetic energy, paramagnetic exchange, and overlap. The integrals are given for the central cell, first neighbor, and second neighbor interactions with only the non-zero ones listed. Short abbreviations are used, such as x^2 for (x^2-y^2) and z^2 for $(3z^2-r^2)$.

Integral	KE+PE (Ry)	Exchange (Ry)	Overlap
	Central Cell (000)		
z^2,z^2	3.098	-3.784	1.000
x^2,x^2	3.098	-3.784	1.000
xy,xy	3.096	-3.784	1.000
yz,yz	3.096	-3.784	1.000
xz,xz	3.096	-3.784	1.000
yz,xz	0.0	0.0	0.0
xy,z^2	0.0	0.0	0.0
	1st Neighbor (110)		
z^2,z^2	-0.006663	-0.005573	0.004558
x^2,x^2	0.01234	0.005775	-0.005819
xy,xy	-0.01681	-0.01608	0.01254
yz,yz	0.005401	0.002811	-0.002626
xz,xz	0.005401	0.002811	-0.002626
yz,xz	0.007073	0.003399	-0.003194

TABLE II (Continued)

xy,z^2	0.008725	0.008919	-0.006911
	2nd Neighbor (002)		
z^2,z^2	-0.001685	-0.0001589	0.0003084
x^2,x^2	-0.00001974	-0.00000306	0.000002427
xy,xy	-0.00001857	-0.000002352	0.000002427
yz,yz	0.0003332	0.0000437	-0.00004984
xz,xz	0.0003332	0.0000437	-0.00004984
yz,xz	0.0	0.0	0.0
xy,z^2	0.0	0.0	0.0

TABLE III

Some Characteristic Energy Differences (Ry)

	Majority Spin	Minority Spin
$\Gamma_{25}-\Gamma_1$	0.506	0.544
$\Gamma_{12}-\Gamma_{25}$	0.084	0.087
X_5-X_1	0.324	0.324
X_5-X_2	0.016	0.017
$X_4'-X_5$	0.144	0.101
$L_2'-L_{32}$	0.016	-0.029
$X_4'-\ _1$	0.807	0.808
$W_1'-W_1$	0.074	0.078
$W_1'-X_5$	$\sim 4 \times 10^{-5}$	$\sim 4 \times 10^{-5}$

TABLE IV

Some Characteristic Spin Splittings (Ry)

$\Gamma_1(\downarrow) - \Gamma_1(\uparrow)$	0.022
$\Gamma_{25}'(\downarrow) - \Gamma_{25}'(\uparrow)$	0.060
$\Gamma_{12}(\downarrow) - \Gamma_{12}(\uparrow)$	0.063
$X_1(\downarrow) - X_1(\uparrow)$	0.054
$X_5(\downarrow) - X_5(\uparrow)$	0.066
$L_{32}(\downarrow) - L_{32}(\uparrow)$	0.065
$L_2'(\downarrow) - L_2'(\uparrow)$	0.020
$X_4'(\downarrow) - X_4'(\uparrow)$	0.023

TABLE V

	Symmetry Axis	Extremal Area (A. U.)	$\frac{m^*}{m_0}$
$L_2'(\uparrow)$ neck	(111)	0.0093	0.09
$X_5(\downarrow)$ hole pocket	(100)	0.020	0.14
	ΓXW plane	0.055	
$X_2(\downarrow)$ hole pocket	(100)	0.061	1.23
	ΓXW plane	0.096	

TABLE VI

Comparison of Two Center Integrals (Ry)

Type	Present Results (α=1)	Fletcher and Wohlfarth[a]	Hodges and Ehrenreich[b]	Zornberg[c]
$dd\sigma$	-0.0428	-0.0248	-0.0384	-0.038
$dd\pi$	0.0186	0.0134	0.0228	0.017
$dd\delta$	-0.0022	-0.0019	0.0056	-0.0017

(a) (1951)

(b) From three center fit to APW calculation (1968).

(c) From two center fit to APW calculation (1970).

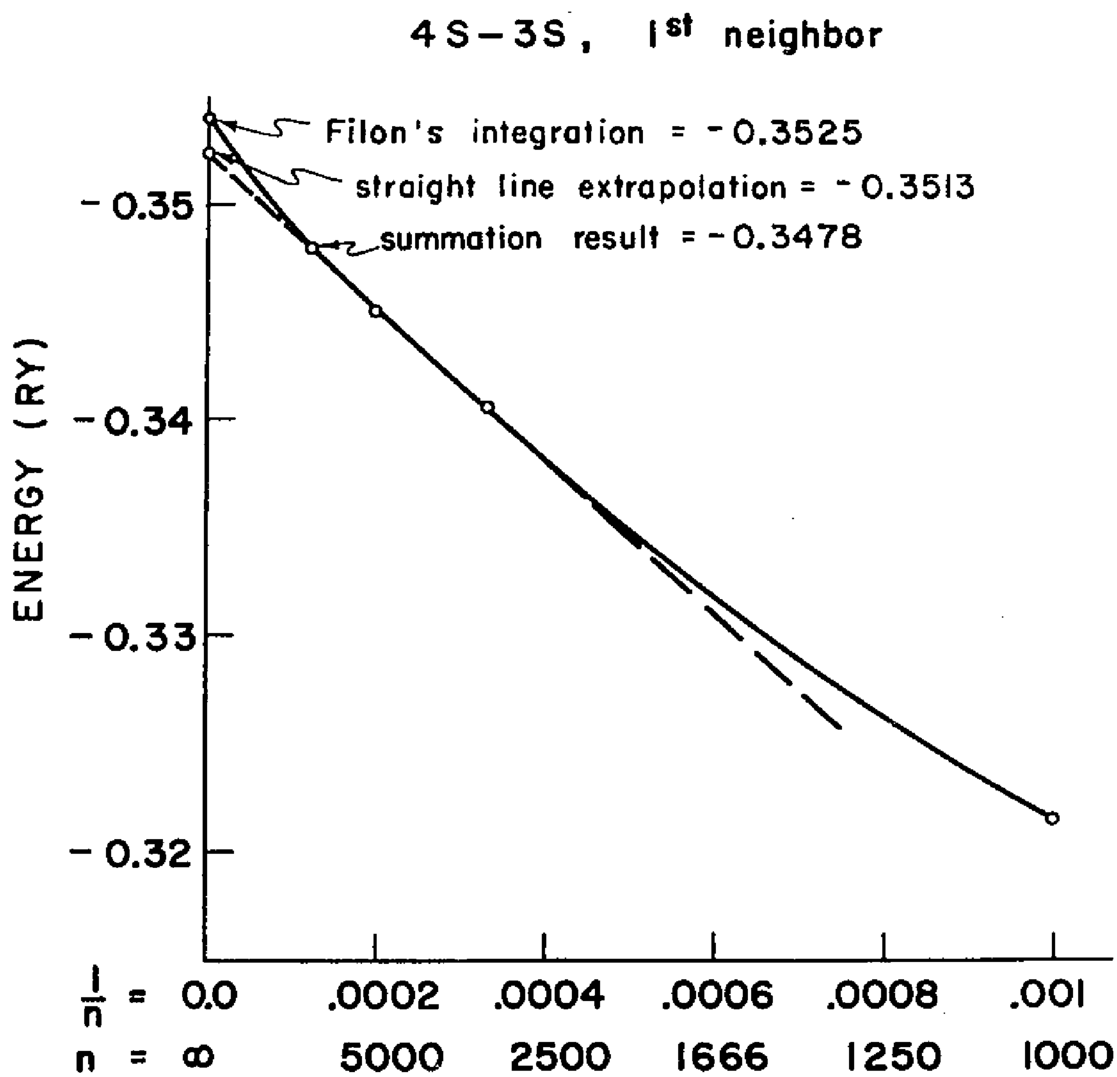
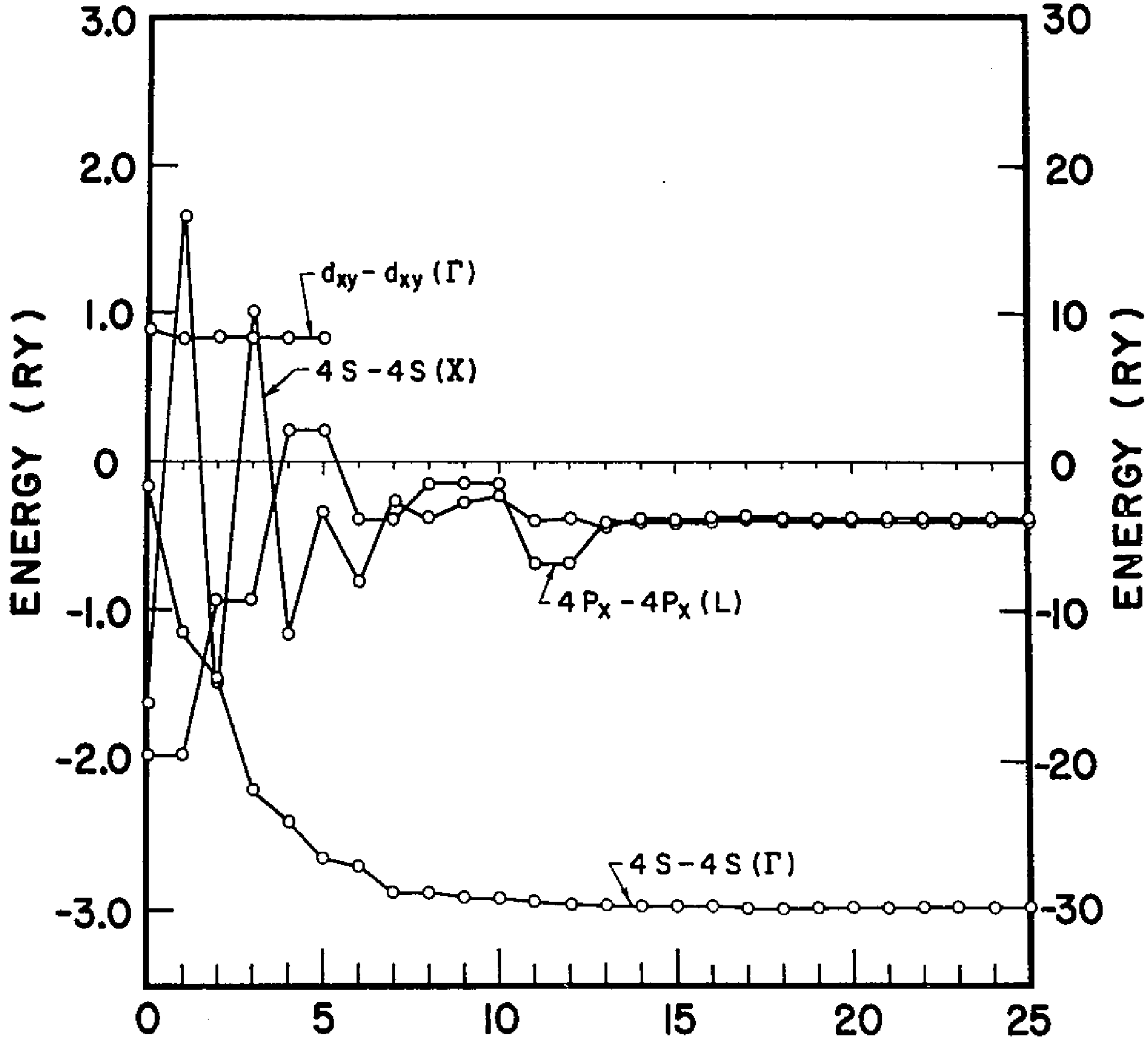

4S−3S, 1st neighbor
Filon's integration = −0.3525
straight line extrapolation = −0.3513
summation result = −0.3478
ENERGY (RY)
−0.35
−0.34
−0.33
−0.32
1/n = 0.0
.0002
.0004
.0006
.0008
.001
n = ∞
5000
2500
1666
1250
1000

FIG. 1



3.0
2.0
1.0
0
-1.0
-2.0
-3.0
ENERGY (RY)
30
20
10
0
-10
-20
-30
ENERGY (RY)
0
5
10
15
20
25
$d_{xy} - d_{xy}$ (Γ)
4 S - 4 S (X)
$4P_x - 4P_x$ (L)
4 S - 4 S (Γ)

FIG. 2

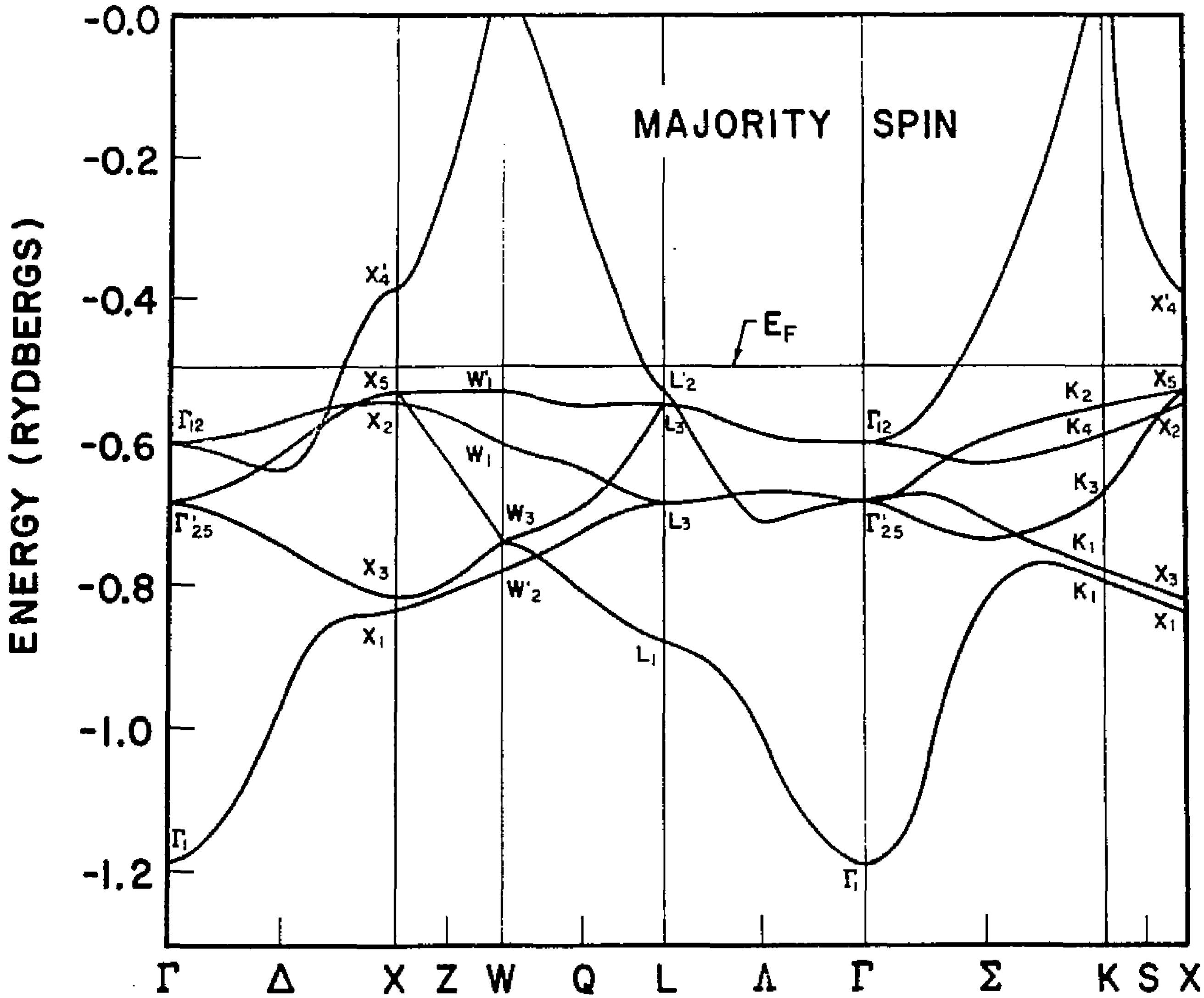
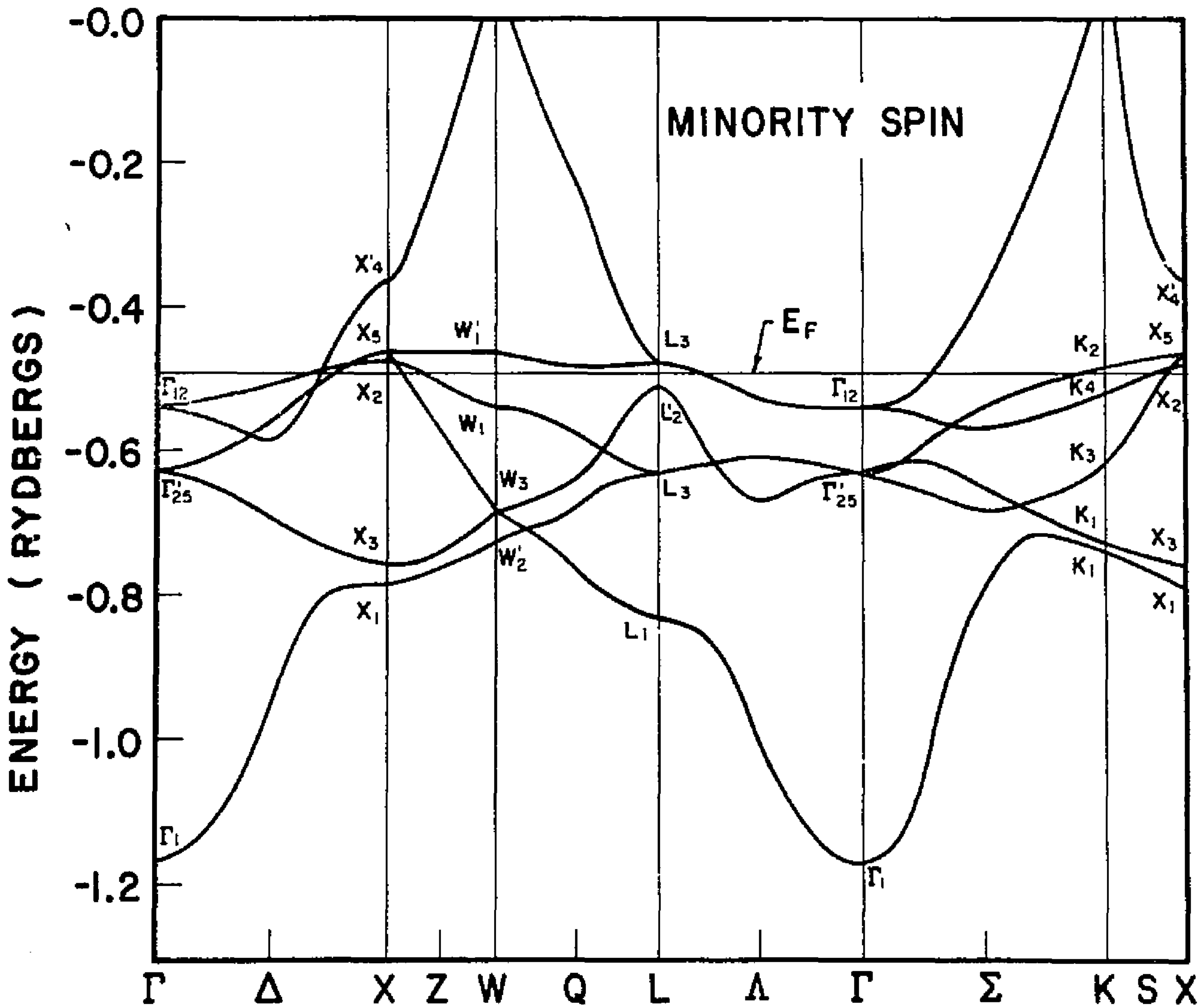

MAJORITY SPIN
ENERGY (RYDBERGS)
-0.0
-0.2
-0.4
-0.6
-0.8
-1.0
-1.2
E_F
Γ Δ X Z W Q L Λ Γ Σ K S X
X'4
X5
X2
X3
X1
W'1
W1
W3
W'2
L'2
L3
L3
L1
Γ12
Γ'25
Γ1
Γ12
Γ'25
Γ1
K2
K4
K3
K1
K1
X'4
X5
X2
X3
X1

FIG. 3



MINORITY SPIN
E_F
ENERGY (RYDBERGS)
-0.0
-0.2
-0.4
-0.6
-0.8
-1.0
-1.2
Γ Δ X Z W Q L Λ Γ Σ K S X
X'_4
X_5
X_2
X_3
X_1
W'_1
W_1
W_3
W'_2
L_3
L'_2
L_1
Γ_{12}
Γ'_{25}
Γ_1
K_2
K_4
K_3
K_1

FIG. 4

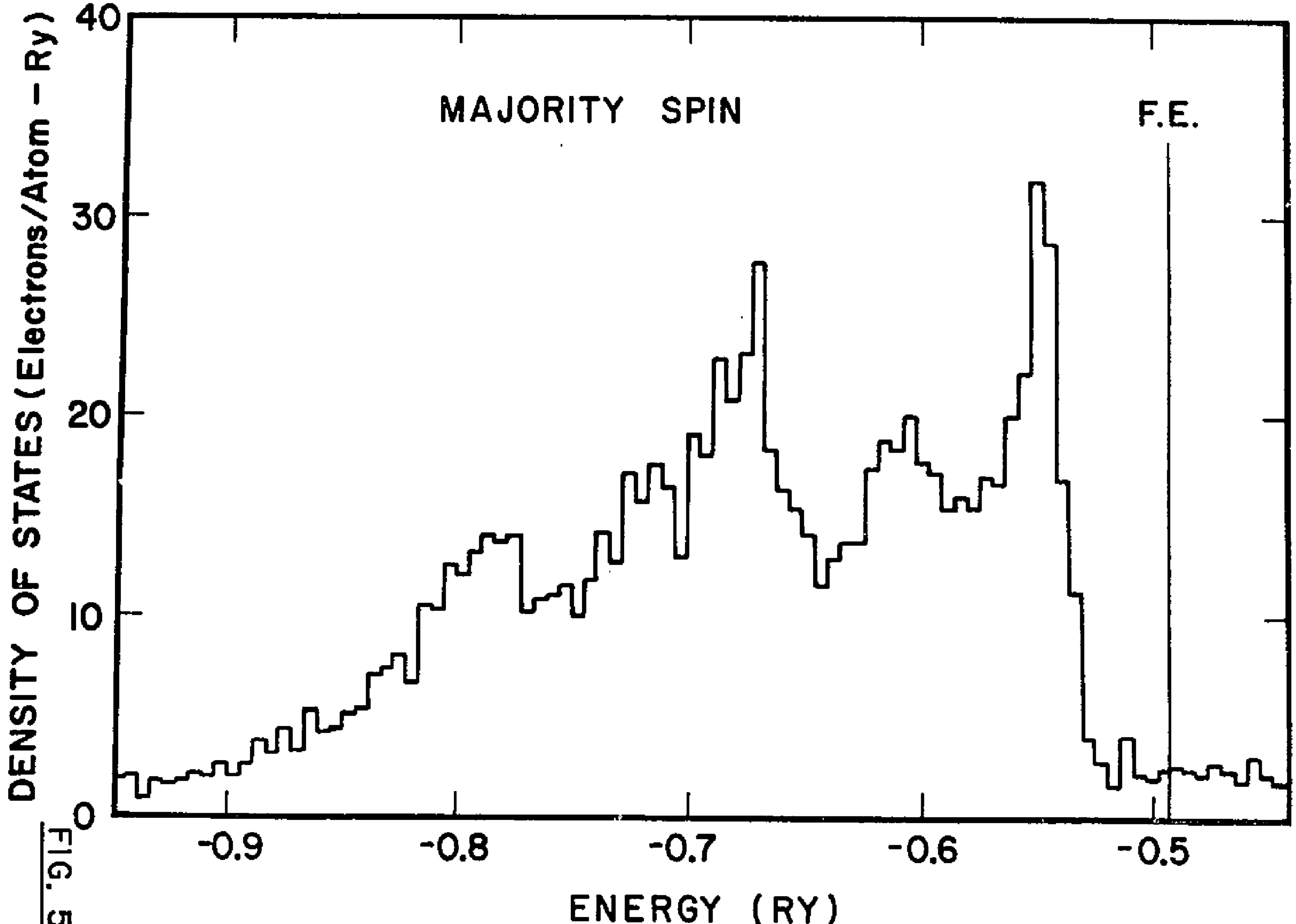

MAJORITY SPIN
F.E.
DENSITY OF STATES (Electrons/Atom - Ry)
0
10
20
30
40
-0.9
-0.8
-0.7
-0.6
-0.5
ENERGY (RY)

FIG. 5

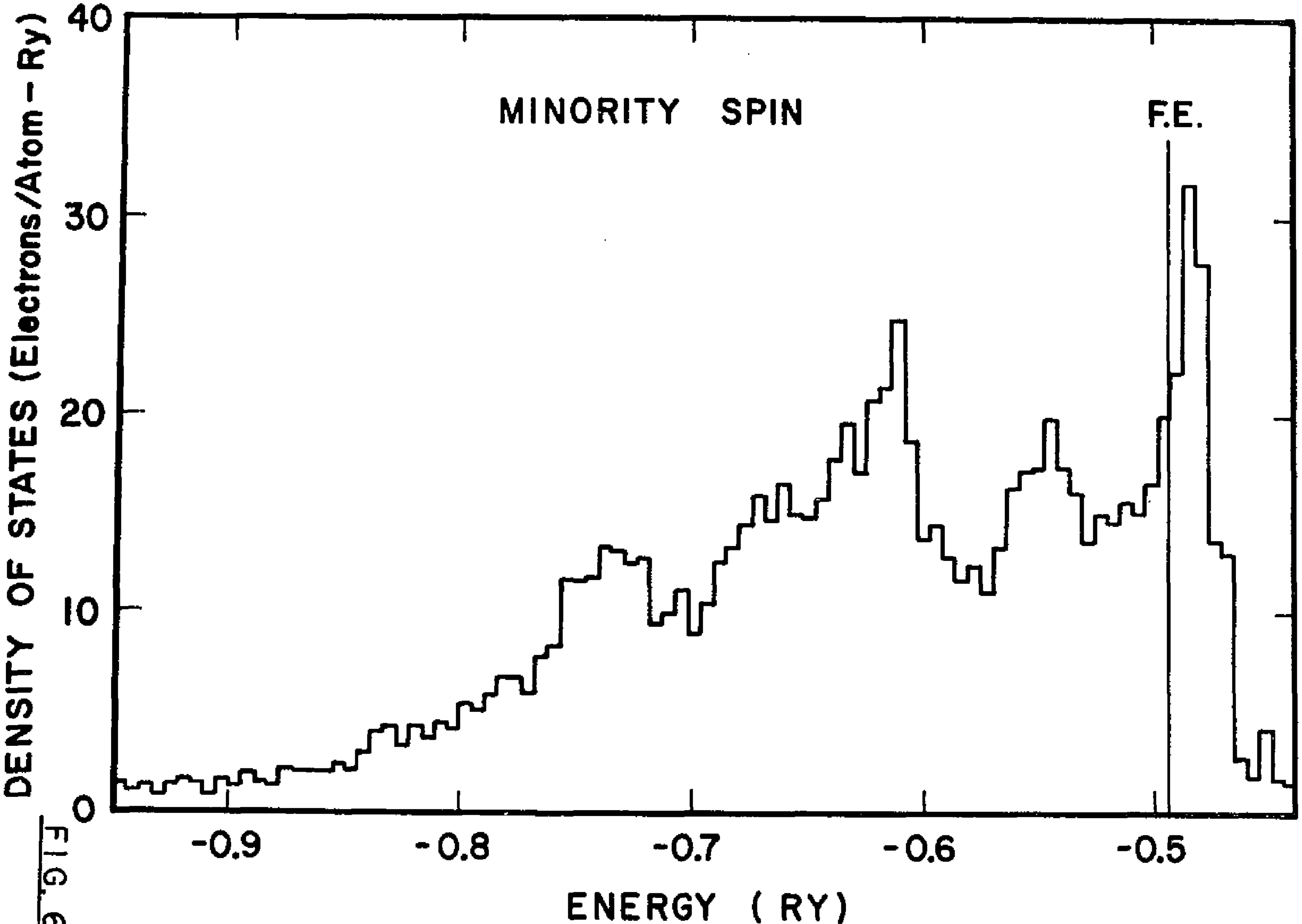

MINORITY SPIN
F.E.
DENSITY OF STATES (Electrons/Atom - Ry)
40
30
20
10
0
-0.9
-0.8
-0.7
-0.6
-0.5
ENERGY (RY)

FIG. 6

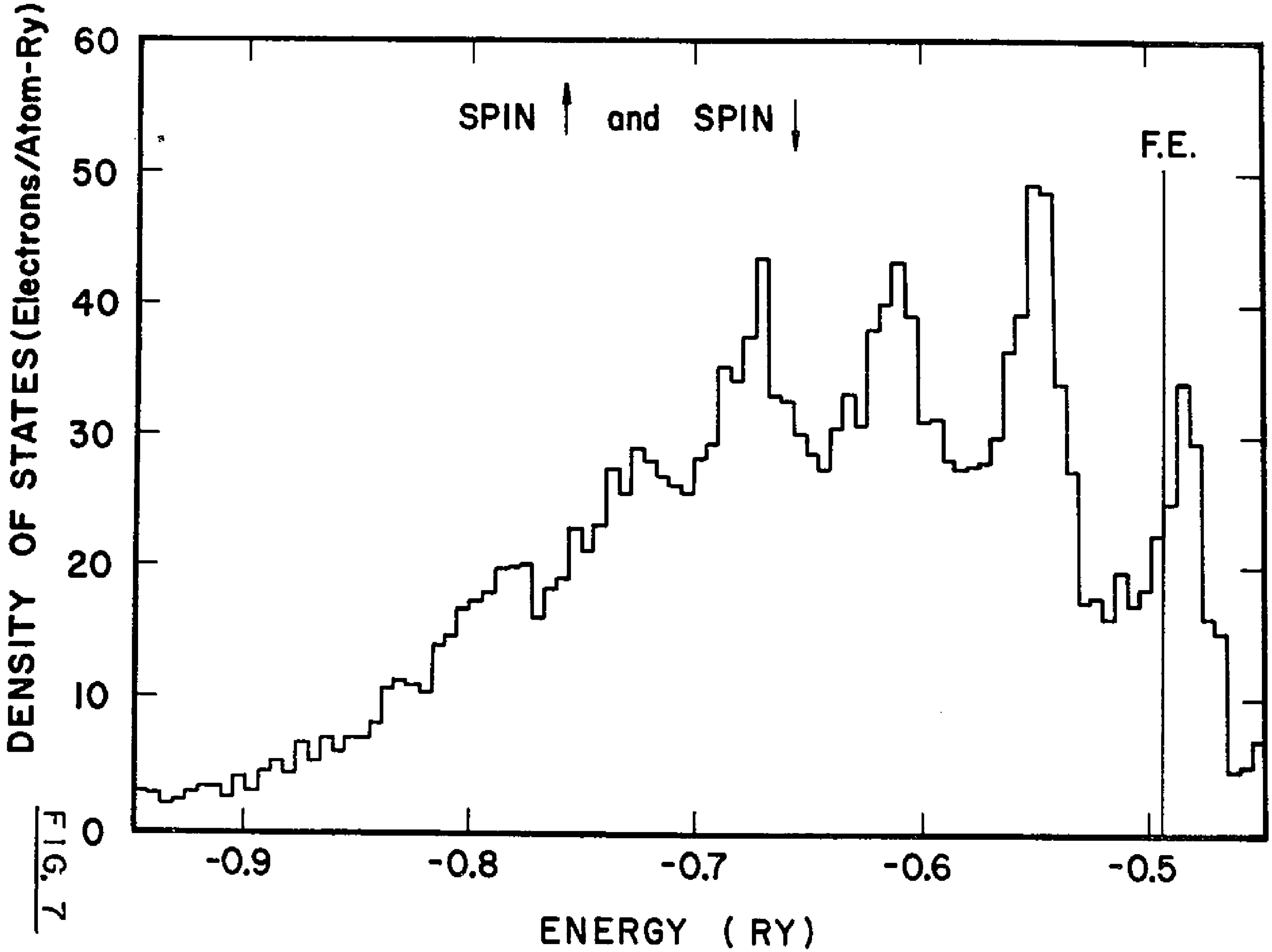

SPIN ↑ and SPIN ↓
F.E.
DENSITY OF STATES (Electrons/Atom-Ry)
ENERGY (RY)
0
10
20
30
40
50
60
-0.9
-0.8
-0.7
-0.6
-0.5

FIG. 7

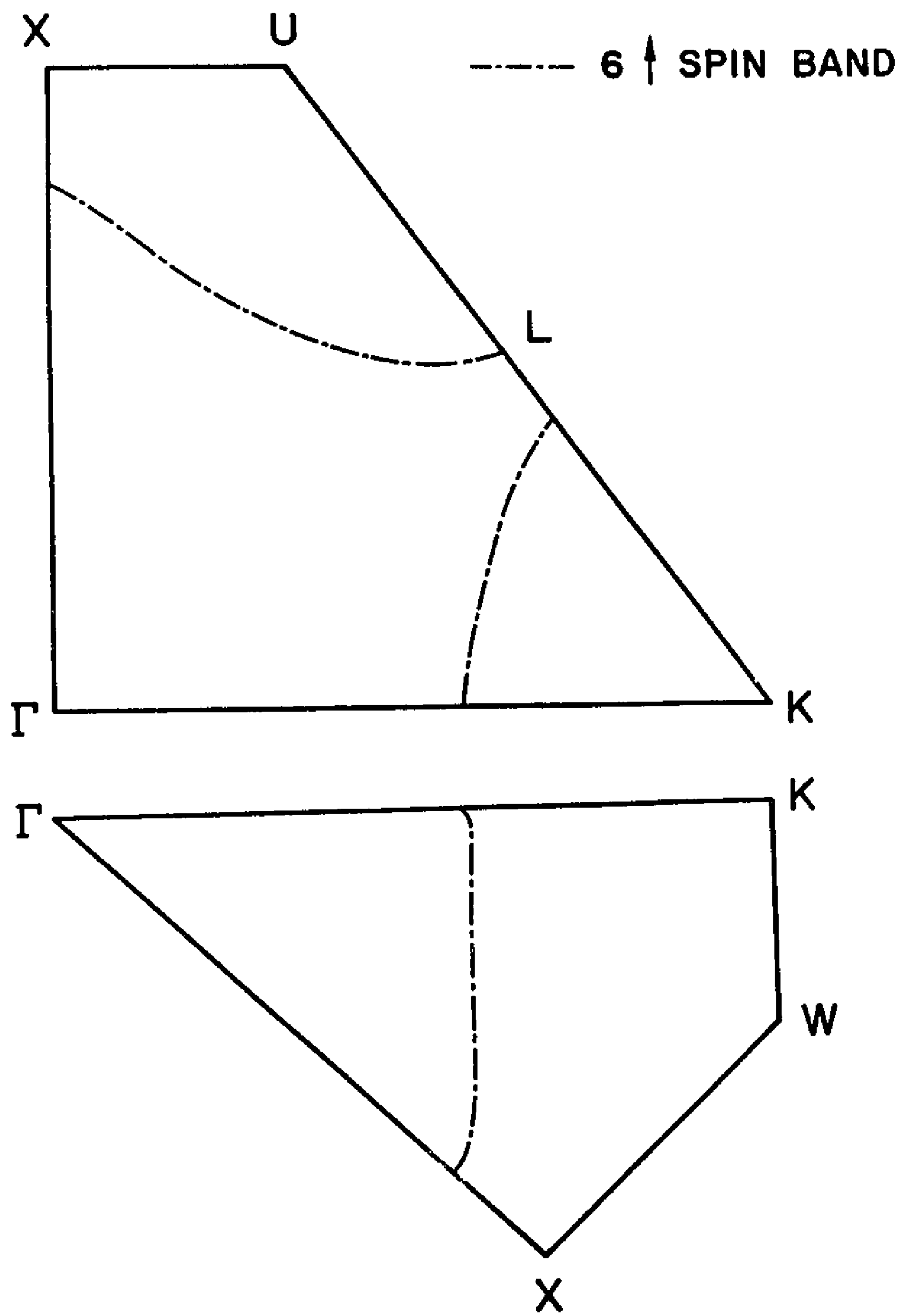


FIG. 8

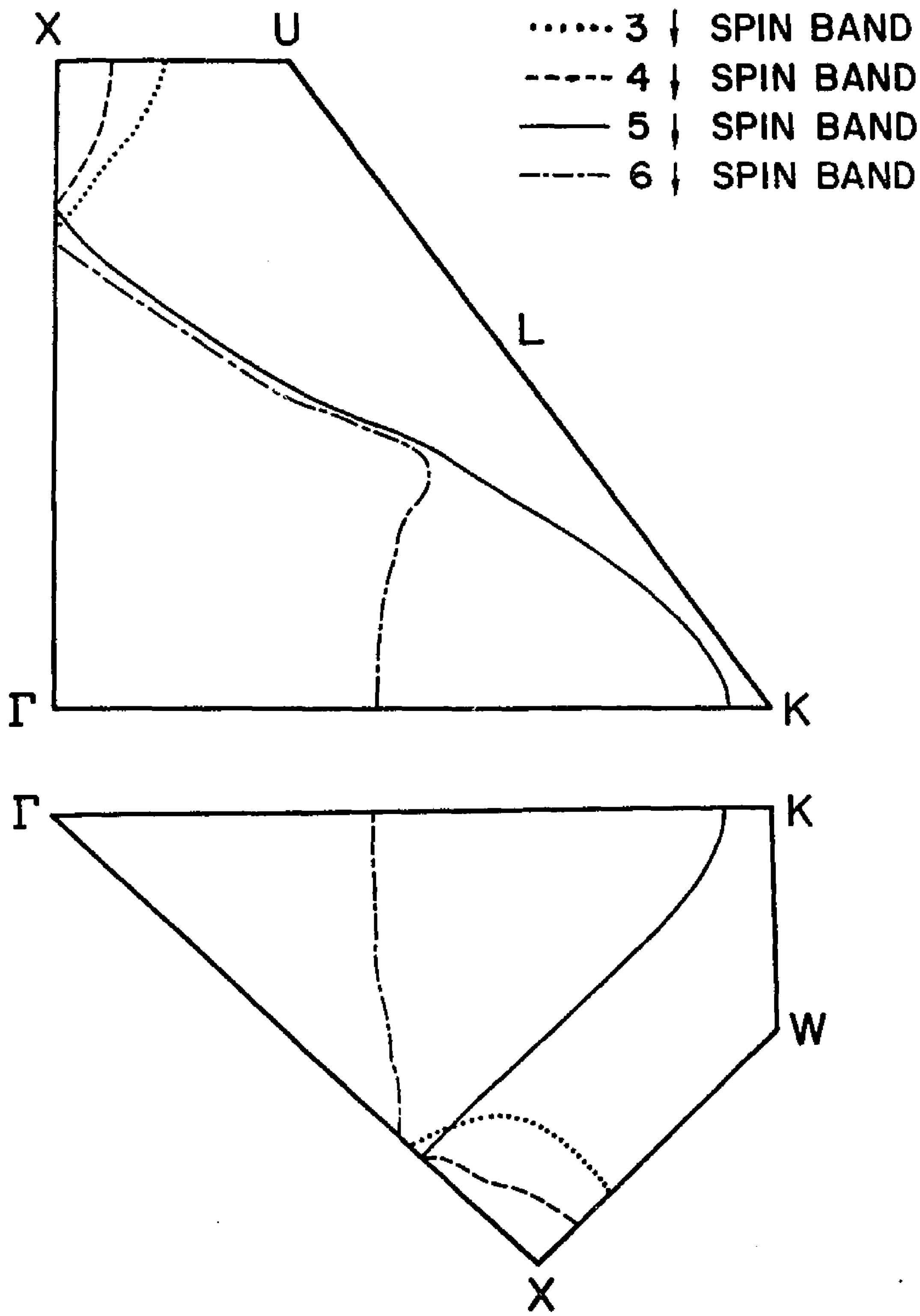


FIG. 9

APPENDIX A

Below are the integral expressions used in the computation of the expectation value of 1 for the overlap, $-\frac{1}{2}\nabla^2$ for the kinetic energy, r^2, and $\cos(\underline{K}_V \cdot \underline{r}_{CD})$, where the wavefunctions are linear combinations of Gaussian-type orbitals, that is, $\exp(-a_1 r^2)$. Only the independent expressions are given. The others can be obtained by cyclic permutations of x,y, and z. We make use of the notation

$$\langle s|s\rangle = \langle G^s(a_1,\underline{r}-\underline{A})|G^s(a_2,\underline{r}-\underline{B})\rangle,$$

and using the definitions

$$\frac{d}{dA_x}\cos(\underline{K}_V \cdot \underline{r}_{CD}) = -K_x u \sin(\underline{K}_V \cdot \underline{r}_{CD})$$

$$\frac{d}{dB_x}\cos(\underline{K}_V \cdot \underline{r}_{CD}) = -K_x(1-u) \sin(\underline{K}_V \cdot \underline{r}_{CD})$$

$$\frac{d}{dA_x}\exp(-LR^2) = 2LX$$

$$\frac{d}{dB_x}\exp(-LR^2) = -2LX$$

we can derive the expressions. The symbols used are defined as

$$u = \frac{a_1}{a_1 + a_2} \qquad E = \exp\left(\frac{K_V{}^2}{4(a_1 + a_2)}\right)$$

$$L = \frac{a_1 a_2}{a_1 + a_2} \qquad W = \frac{1}{a_1 + a_2}$$

$$D = \left[\frac{\pi}{a_1 + a_2}\right]^{3/2} \qquad T = \exp(-LR^2)$$

$$X = B_x - A_x \qquad Y = B_y - A_y$$

$$Z = B_z - A_z \qquad R^2 = X^2 + Y^2 + Z^2$$

$$\cos = \cos(\underline{K}_V \cdot \underline{r}_{CD}) \qquad \sin = \sin(\underline{K}_V \cdot \underline{r}_{CD})$$

$K_x = K_{vx}$

The constants below are the numerical factors involved in the spherical harmonics associated with the electron state wavefunctions.

$C_1 = 0.07957747$	$C_2 = 0.13783228$
$C_3 = 0.23873262$	$C_6 = 0.08897035$
$C_5 = 0.15410117$	$C_4 = 0.30820235$
$C_9 = 0.15410111$	$C_8 = 0.26691118$
$C_7 = 0.53382235$	$C_{15} = 0.09947184$
$C_{14} = 0.17229028$	$C_{13} = 0.34458056$
$C_{12} = 0.29841552$	$C_{11} = 0.59683104$
$C_{10} = 1.19366207$	

We can derive all subsequent integrals from $\langle s|0|s\rangle$, where 0 is one of the operators, $-\frac{1}{2}\nabla^2$ or cos $\underline{K}_v \cdot \underline{r}_{CD}$. Some are shown as follows:

$$\langle P_x|0|s\rangle = \frac{1}{2a_1}\frac{d}{dA_x}\langle s|0|s\rangle$$

$$\langle P_x|0|P_x\rangle = \frac{1}{2a_2}\frac{d}{dB_x}\langle P_x|0|s\rangle = \frac{1}{2a_1}\frac{d}{dA_x}\frac{1}{2a_2}\frac{d}{dB_x}\langle s|0|s\rangle$$

$$d_{xy}\ 0\ s = \frac{1}{2a_1}\frac{d}{dA_y}\ P_x\ 0\ s = \frac{1}{2a_1}\frac{d}{dA_y}\frac{1}{2a_2}\frac{d}{dA_x}\ s\ 0\ s$$

$$\langle d_{(x^2-y^2)}|0|s\rangle = \frac{1}{2a_1}\frac{d}{dA_x}\langle P_x|0|s\rangle - \frac{1}{2a_1}\frac{d}{dA_y}\langle P_y|0|s\rangle$$

$$\langle d_{(3z^2-r^2)}|0|s\rangle = \langle d_{(2z^2-x^2-y^2)}|0|s\rangle$$

$$= \frac{1}{a_1}\frac{d}{dA_z}\langle P_z|0|s\rangle - \frac{1}{2a_1}\frac{d}{dA_x}\langle P_x|0|s\rangle - \frac{1}{2a_1}\frac{d}{dA_y}\langle P_y|0|s\rangle$$

KINETIC ENERGY INTEGRALS

$$\langle s|-\nabla^2|s\rangle = 2C_1DTL(3-2LR^2)$$

$$\langle p_x|-\nabla^2|s\rangle = 2C_2DTLWa_2X(5-2LR^2)$$

$$\langle p_x|-\nabla^2|p_x\rangle = 2C_3DTLW(2.5-7LX^2-LR^2+2L^2X^2R^2)$$

$$\langle p_x|-\nabla^2|p_y\rangle = 2C_3DTL^2WXY(2LR^2-7)$$

$$\langle d_{xy}|-\nabla^2|s\rangle = 2C_4DTLW^2a_2^2XY(7-2LR^2)$$

$$\langle d_{(x^2-y^2)}|-\nabla^2|s\rangle = 2C_5DTLW^2a_2^2(X^2-Y^2)(7-2LR^2)$$

$$\langle d(3_z{}^2-r^2)|-\nabla^2|s\rangle = 2C_6DTLW^2a_2^2(2Z^2-X^2-Y^2)(7-2LR^2)$$

$$\langle d_{xy}|-\nabla^2|p_x\rangle = 2C_7DTLW^2a_1Y(3.5-9LX^2-LR^2+2L^2X^2R^2)$$

$$\langle d_{xy}|-\nabla^2|p_z\rangle = 2C_7DTW^3La_1a_2^2XYZ(2\ R^2-9)$$

$$\langle d(x^2-y^2)|-\nabla^2|p_x\rangle = 2C_8DTLW^2a_2X(7-2LR^2 \\ +(Y^2-X^2)(9L-2L^2R^2))$$

$$\langle d_{(x^2-y^2)}|-\nabla^2|p_y\rangle = 2C_8DTLW^2a_2Y(-7+2LR^2 \\ +(Y^2-X^2)(9L-2L^2R^2)$$

$$\langle d_{(x^2-y^2)}|-\nabla^2|p_z\rangle = 2C_8DTLW^2a_2Z(Y^2-X^2)(9L-2L^2R^2)$$

$$\langle d_{(3_z{}^2-r^2)}|-\nabla^2|p_x\rangle = 2C_9DTLW^2a_2X(2LR^2-7 \\ +(X^2+Y^2-2Z^2)(9L-2L^2R^2))$$

$$\langle d_{(3_z{}^2-r^2)}|-\nabla^2|p_z\rangle = 2C_9DTLW^2a_2Z(2(7-2LR^2) \\ +(X^2+Y^2-2Z^2)(9L-2L^2R^2))$$

$$\langle d_{xy}|-\nabla^2|d_{xy}\rangle = 2C_{10}DTLW^2((3.5-9LY^2)(1-2LX^2) \\ +(2L^2Y^2-L)(2X^2+R^2-2LX^2R^2))$$

$$\langle d_{yz}|-\nabla^2|d_{xy}\rangle = 2C_{10}DTL^2W^2XZ(-4.5+11LY^2+LR^2-2L^2Y^2R^2)$$

$$\langle d_{yz}|-\nabla^2|d_{yz}\rangle = 2C_{10}DTLW^2((3.5-9LY^2)(1-2LZ^2) \\ +(2L^2Y^2-L)(2Z^2+R^2-2LZ^2R^2))$$

$$\langle d_{zx}|-\nabla^2|d_{xy}\rangle = 2C_{10}DTL^2W^2YZ(11LX^2-4.5+LR^2-2L^2X^2R^2)$$

$$\langle d_{zx}|-\nabla^2|d_{yz}\rangle = 2C_{10}DTL^2W^2XY(11LX^2-4.5+LR^2-2L^2Z^2R^2)$$

$$\langle d_{zx}|-\nabla^2|d_{zx}\rangle = 2C_{10}DTLW^2((3.5-9LZ^2)(1-2LX^2) +(2L^2Z^2-L)(2X^2+R^2-2LX^2R^2))$$

$$\langle d_{(x^2-y^2)}|-\nabla^2|d_{xy}\rangle = 2C_{11}DTL^3W^2XY(X^2-Y^2)(11-2LR^2)$$

$$\langle d_{(x^2-y^2)}|-\nabla^2|d_{yz}\rangle = 2C_{11}DTL^2W^2YZ(9-2LR^2 +(X^2-Y^2)(11L-2L^2R^2))$$

$$\langle d_{(x^2-y^2)}|-\nabla^2|d_{zx}\rangle = 2C_{11}DTL^2W^2XZ(-9+2LR^2 +(X^2-Y^2)(11L-2L^2R^2))$$

$$\langle d_{(x^2-y^2)}|-\nabla^2|d_{(x^2-y^2)}\rangle = 2C_{12}DTLW^2(7 +(X^4+Y^4)(11L^2-2L^3R)-2LR +(X^2+Y^2)(4L^2R-18L) +X^2Y^2(4L^3R-22L^2))$$

$$\langle d_{(3_z{}^2-r^2)}|-\nabla^2|d_{xy}\rangle = 2C_{13}DTL^2W^2XY(18-4LR^2 +(X^2+Y^2-2Z^2)(2L^2R^2-11L))$$

$$\langle d_{(3_z{}^2-r^2)}|-\nabla^2|d_{yz}\rangle = 2C_{13}DTL^2W^2YZ(-9+2LR^2 +(X^2+Y^2-2Z^2)(2L^2R^2-11L))$$

$$\langle d_{(3_z{}^2-r^2)}|-\nabla^2|d_{(x^2-y^2)}\rangle = 2C_{14}DTL^2W^2(X^2-Y^2) ((X^2+Y^2-2Z^2)(2L^2R^2-11L) -2(9-2LR^2))$$

$$\langle d_{(3_z{}^2-r^2)}|-\nabla^2|d_{(3_z{}^2-r^2)}\rangle = 2C_{15}DTLW^2(21-6LR^2 -2(9L-2L^2R^2)(X^2+Y^2+4Z^2) +(X^2+Y^2-2Z^2)^2(11L^2-2L^3R^2))$$

r^2 Integrals

$\langle s|r^2|s\rangle = DTW(1.5+a_2^2WR^2)$

$\langle P_x|r^2|s\rangle = DTW^2Xa_2(2.5+a_2^2WR^2)$

$\langle P_x|r^2|P_x\rangle = DTW^2((\frac{1}{2}-LX^2)(2.5+a_2^2WR^2)\ +a_2^2WX^2)$

$\langle P_x|r^2|P_y\rangle = DTWLXY(1.5+a_2^2WR^2+a_2W(2u-1))$

$\langle d_{xy}|r^2|s\rangle = DTW3a_2^2XY(3.5+a_2^2WR^2)$

$\langle d(x^2-y^2)|r^2|s\rangle = DTW^3a_2^2(X^2-Y^2)(3.5+a_2^2WR^2)$

$\langle d(3_z{}^2-r^2)|r^2|s\rangle = DTW^3a_2^2(3Z^2-R^2)(3.5+a_2^2WR^2)$

$\langle d_{xy}|r^2|P_x\rangle = \frac{1}{2}DTW^3a_2^2(W(Y/L-2X^2Y)(3.5a_1-a_2\ +a_1a_2^2WR^2)$
$\quad +Y/a_1)$

$\langle d_{xy}|r^2|P_z\rangle = DTW^4a_2^2XYZ(a_2-3.5a_1-a_1a_2^2WR^2)$

$\langle d(x^2-y^2)|r^2|P_x\rangle = DTW3a_2(a_2^2WX(X^2-Y2)$
$\quad +X(1.0-L(X^2-Y^2))(3.5+a_2^2WR^2))$

$\langle d(x^2-y^2)|r^2|P_z\rangle = -DTW^4a_2^2Z(X^2-Y^2)(3.5a_1-a_2+a_1a_2^2WR^2)$

$\langle d(3_z{}^2-r^2)|r^2|P_x\rangle = DTW3a_2((L(X^2-Y^2-2Z^2)-X)$
$\quad (3.5+a_2^2WR^2)-a_2^2W(X^2+Y^2-2Z^2))$

$\langle d(3_z{}^2-r^2)|r^2|P_z\rangle = DTW^3a_2(Z(2+L(X^2+Y^2-2Z^2))(3.5+\ {}_2{}^2WR^2)$
$\quad -ZWa_2^2(X^2+Y^2-2Z^2))$

$\langle d_{xy}|r^2|d_{xy}\rangle = \frac{1}{4}DTW^4a_2((1-2LY^2)(1/\ -2X^2)(3.5a_1-a_2+a_1a_2^2WR^2)$
$\quad +a_2^2W(1/\ 2-4X^2Y^2))$

$\langle d_{xy}|r^2|d_{xz}\rangle = \frac{1}{2}DTW^4a_2(YZ(2LX^2-1)(3.5a_1-a_2+a_1a_2^2WR^2)$
$\quad -2a_1Wa_2^2X^2YZ)$

$$\langle d_{yz}|r^2|d_{(x^2-y^2)}\rangle = DTW^4a_2((1+LYZ(X^2-Y^2))(3.5a_1-a_2+a_1a_2^2WR^2) -a_1a_2^2WYZ(X^2-Y^2))$$

$$\langle d_{xy}|r^2|d_{(x^2-y^2)}\rangle = DTW^5a_1a_2^2XY(X^2-Y^2)(a_1(3.5+a_2^2WR^2)-2a_2)$$

$$\langle d_{xz}|r^2|d_{(3_z{}^2-r^2)}\rangle = DTW^4a_2XZ((1+L(X^2+Y^2-2Z^2)) (a_2-3.5a_1-a_1a_2^2WR^2)+a_1a_2^2W(X^2+Y^2-2Z^2))$$

$$\langle d_{xy}|r^2|d_{(3_z{}^2-r^2)}\rangle = DTW^4a_2XY((2- \quad (X^2+Y^2-2Z^2)) (3.5a_1-a_2+a_1a_2^2WR^2)+a_1a_2^2W(X^2+Y^2-2Z^2))$$

$$\langle d_{(x^2-y^2)}|r^2|d_{(x^2-y^2)}\rangle = DTW3((1-2L(X^2+Y^2)+L^2(X^2-Y^2)^2) (3.5+a_2^2WR^2)+2a_2^2W(X^2+Y^2-L(X^2-Y^2)^2))$$

$$\langle d_{(x^2-y^2)}|r^2|d_{(3_z{}^2-r^2)}\rangle = DTW^4a_2(X^2-Y^2)((2-L(X^2+Y^2-2Z^2) (3.5a_1-a_2+a_1a_2^2WR^2) +a_1a_2^2W(X^2+Y^2-2Z^2))$$

$$\langle d_{(3_z{}^2-r^2)}|r^2|d_{(3_z{}^2-r^2)}\rangle = \tfrac{1}{4}DTW^4a_2((12/L-8(4Z^2+X^2+Y^2) +4L(X^2+Y^2-2Z^2)(X^2+Y^2-2Z^2)) (3.5a_1-a_2+a_1a_2^2WR^2) +a_1a_2^2W(12/L^2-4(X^2+Y^2-2Z^2) (X^2+Y^2-2Z^2)))$$

$\cos(K_v \cdot r_{CD})$ INTEGRALS

$$\langle s|\cos|s\rangle = C_1 DTE \cos$$

$$\langle P_x|\cos|s\rangle = C_2 DTEW(a_2 X\cos - \tfrac{1}{2}K_x \sin)$$

$$\langle P_x|\cos|P_x\rangle = C_3 DTEW((\tfrac{1}{2} - LX^2 - \tfrac{1}{4}WK_x^2)\cos + \tfrac{1}{2}XK_x(2u-1)\sin)$$

$$\langle P_x|\cos|P_y\rangle = C_3 DTEW^2(\tfrac{1}{2}(a_1K_xY - a_2K_yX)\sin - (a_1a_2XY + \tfrac{1}{4}K_xK_y)\cos)$$

$$\langle d_{xy}|\cos|s\rangle = C_4 DTEW^2((a_2^2XY - \tfrac{1}{4}K_xK_y)\cos - \tfrac{1}{2}a_2(YK_x + XK_y)\sin)$$

$$\langle d_{(x^2-y^2)}|\cos|s\rangle = C_5 DTEW^2((a_2^2(X^2-Y^2) - \tfrac{1}{4}(K_x^2 - K_y^2))\cos$$
$$-a_2(XK_x - YK_y)\sin$$

$$\langle d_{(3z^2-r^2)}|\cos|s\rangle = C_6 DTEW^2(\cos(a_2^2(2Z^2 - X^2 - Y^2)$$
$$-\tfrac{1}{4}(2K_z^2 - K_x^2 - K_y^2)) - a_2(2ZK_z - XK_x - YK_y)\sin)$$

$$\langle d_{xy}|\cos|P_x\rangle = C_7 DTEW^2(\cos(\tfrac{1}{4}XK_xK_y(2u-1) + \tfrac{1}{2}a_2Y$$
$$-\tfrac{1}{4}a_2K_x^2WY - a_2LX^2Y) - \sin(\tfrac{1}{2}a_2K_xXY(1-2u)$$
$$+\tfrac{1}{4}K_y - \tfrac{1}{2}LX^2K_y - K_yK_x^2W/8))$$

$$\langle d_{xy}|\cos|P_z\rangle = C_7 DTEW3(\cos(-\tfrac{1}{4}a_2K_z(XK_y - YK_x) + a_1Z(\tfrac{1}{4}K_xK_y - a_2^2XY))$$
$$-\tfrac{1}{2}\sin(K_z(a_2^2XY - \tfrac{1}{4}K_xK_y) - a_1a_2Z(XK_y + YK_x)))$$

$$\langle d_{(x^2-y^2)}|\cos|P_x\rangle = C_8 DTEW^3(\cos(a_1X(\tfrac{1}{4}(K_x^2 - K_y^2 - a_2^2(X^2 - Y^2))$$
$$-\tfrac{1}{2}a_2K_x(XK_x - YK_y) + a_2X/W)$$
$$-\sin(-a_1a_2Y(XK_x - YK_y) + \tfrac{1}{2}K_y(a_2^2(X^2 - Y^2)$$
$$-\tfrac{1}{4}(K_x^2 - K_y^2) - 1/W)))$$

$$\langle d_{(x^2-y^2)}|\cos|P_y\rangle = C_8 DTEW^3(\cos(a_1Y(\tfrac{1}{4}(K_x^2 - K_y^2) - a_2^2(X^2 - Y^2))$$
$$-\tfrac{1}{2}a_2K_y(XK_x - YK_y) - a_2Y/W)$$
$$-\sin(-a_1a_2Y(XK_x - YK_y) + \tfrac{1}{2}K_y(a_2^2(X^2 - Y^2)$$
$$-\tfrac{1}{4}(K_x^2 - K_y^2) - 1/W)))$$

$$\langle d_{(x^2-y^2)}|\cos|P_z\rangle = C_8 DTEW^3(\cos(a_1 Z(\tfrac{1}{4}(K_x{}^2-K_y{}^2)$$
$$-a_2^2(X^2-Y^2))-\tfrac{1}{2}a_2K_z(XK_x-YK_y))$$
$$-\sin(\tfrac{1}{2}K_z(a_2^2(X^2-Y^2)-\tfrac{1}{4}(K_x{}^2-K_y{}^2))$$
$$-a_1a_2Z(XK_x-YK_y)))$$

$$\langle d_{(3_z{}^2-r^2)}|\cos|P_x\rangle = C_9 DTEW^3(\cos(\tfrac{1}{4}a_1X(2K_z{}^2-K_x{}^2-K_y{}^2)$$
$$-a_2^2a_1X(2Z^2-X^2-Y^2)-\tfrac{1}{2}a_2K_x(2ZK_z-XK_x-YK_y)$$
$$-a_2X/W)-\sin(-\tfrac{1}{2}K_x/W-K_x(2K_z{}^2-K_x{}^2-K_y{}^2)/8$$
$$+\tfrac{1}{2}K_xa_2^2(2Z^2-X^2-Y^2)$$
$$-a_1a_2X(2ZK_z-XK_x-YK_y)))$$

$$\langle d_{(3_z{}^2-r^2)}|\cos|P_z\rangle = C_9 DTEW3(\tfrac{1}{4}a_1Z(2K_z{}^2-K_x{}^2-K_y{}^2)$$
$$-a_1a_2^2Z(2Z^2-X^2-Y^2)-\tfrac{1}{2}a_2K_z(2ZK_z-XK_x-YK_y)$$
$$+2a_2Z/W)-\sin(K_z/W+\tfrac{1}{2}a_2^2K_z(2Z^2-X^2-Y^2)$$
$$-K_z(2K_z{}^2-K_x{}^2-K_y{}^2)/8$$
$$-a_1a_2Z(2ZK_z-XK_x-YK_y)))$$

$$\langle d_{xy}|\cos|d_{xy}\rangle = C_{10}DTEW3(\cos(a_1a_2LX^2Y^2 + \tfrac{1}{4}L(Y^2K_x{}^2+X^2K_y{}^2)$$
$$-\tfrac{1}{4}W(a_1-a_2)^2XYK_xK_y - (K_x{}^2+K_y{}^2)/8$$
$$-\tfrac{1}{2}a_1a_2(X^2+Y^2) + K_x{}^2K_y{}^2W/16 + 1/4W)$$
$$+\tfrac{1}{2}(a_2-a_1)\ \sin((YK_x+XK_y)(LXY+\tfrac{1}{4}WK_xK_y)$$
$$-\tfrac{1}{2}(XK_x+YK_y)))$$

$$\langle d_{zx}|\cos|d_{xy}\rangle = C_{10}DTEW^3(\cos(a_1a_2LX^2YZ + \tfrac{1}{4}L(K_x{}^2YZ+X^2K_yK_z)$$
$$+\tfrac{1}{4}(1-2u)XK_x(a_2ZK_y-a_1YK_z) - K_yK_z/8$$
$$-\tfrac{1}{2}a_1a_2YZ + K_x{}^2K_yK_zW/16)$$
$$+ \sin(\tfrac{1}{2}L((a_2-a_1)XK_xYZ + a_2K_yX^2Z$$
$$-a_1X^2YK_z) + \tfrac{1}{2}(a_1YK_z-a_2ZK_y)(\tfrac{1}{2}-\tfrac{1}{4}WK_x{}^2)$$
$$+W(a_2-a_1)XK_xK_yK_z/8))$$

$$\langle d_{xy}|\cos|d_{(x^2-y^2)}\rangle = C_{11}DTEW^3(\cos(a_1(X^2-Y^2)(a_2LXY +$$
$$\tfrac{1}{2}W(a_2-\tfrac{1}{2}a_1)K_xK_y) + W(K_x{}^2-K_y{}^2)(K_xK_y/16$$
$$+ \tfrac{1}{2}a_2(a_1-\tfrac{1}{2}a_2)XY)) + \sin((a_2LXY$$
$$- \tfrac{1}{4}a_1WK_xK_y)(XK_x-YK_y) + (a_2W(K_x{}^2-K_y{}^2)/8$$
$$- \tfrac{1}{2}a_1L(X^2-Y^2))(XK_y + YK_x)$$
$$+ \tfrac{1}{2}(a_1+a_2)(XK_y-YK_x)))$$

$$\langle d_{zx}|\cos|d_{(x^2-y^2)}\rangle = C_{11}DTEW^3(\cos(a_1a_2XZ(X^2-Y^2)-1)$$
$$- \tfrac{1}{4}a_2{}^2WXZ(K_x{}^2-K_y{}^2) - \tfrac{1}{4}a_1{}^2WK_xK_z(X^2-Y^2)$$
$$+ \tfrac{1}{2}L(XK_x-YK_y)(XK_z+ZK_x)$$
$$+ \tfrac{1}{4}K_xK_z(\tfrac{1}{4}W(K_x{}^2-K_y{}^2)-1))$$
$$+ \sin((XK_z+ZK_x)(a_2W(K_x{}^2-K_y{}^2)/8$$
$$- \tfrac{1}{2}a_1L(X^2-Y^2)+(XK_x-YK_y)(a_2LXZ-\tfrac{1}{4}a_1WK_xK_z)$$
$$+ \tfrac{1}{2}(a_1XK_z-a_2ZK_x)))$$

$$\langle d_{zx}|\cos|d_{(3z^2-r^2)}\rangle = C_{13}DTEW^3(\cos(-a_1a_2XZ-\tfrac{1}{4}K_xK_z$$
$$+ (2Z^2-X^2-Y^2)(a_1a_2XZL-\tfrac{1}{4}a_1{}^2WK_xK_z)$$
$$+ \tfrac{1}{4}W(2K_z{}^2-K_x{}^2-K_y{}^2)(\tfrac{1}{4}K_xK_z-a_2{}^2XZ)$$
$$+ \tfrac{1}{2}L(XK_z+ZK_x)(2ZK_z-XK_x-YK_y))$$
$$+ \sin(\tfrac{1}{2}Wa_2(XK_z+ZK_x)(\tfrac{1}{4}(2K_z{}^2-K_x{}^2-K_y{}^2)$$
$$- a_1{}^2(2Z^2-X^2-Y^2))-(a_2+\tfrac{1}{2}a_1)XK_z$$
$$+ (a_1+\tfrac{1}{2}a_2)ZK_x+(2ZK_z-XK_x-YK_y)$$
$$(a_2LXZ-\tfrac{1}{4}Wa_1K_xK_z)))$$

$$\langle d_{(x^2-y^2)}|\cos|d_{(x^2-y^2)}\rangle = C_{12}DTEW^4(\cos(a_1^2a_2^2(X^2-Y^2)^2$$
$$-\tfrac{1}{4}(a_1^2+a_2^2)(X^2-Y^2)(K_x{}^2-K_y{}^2)$$
$$+a_1a_2(XK_x-YK_y)^2-2a_1a_2(X^2+Y^2)/W$$
$$+(K_x{}^2-K_y{}^2)^2\ /16-\tfrac{1}{2}(K_x{}^2+K_y{}^2)/W$$
$$+1/W^2)+\sin((a_2-a_1)(XK_x-YK_y)$$
$$(a_1a_2(X^2-Y^2)+\tfrac{1}{4}(K_x{}^2-K_y{}^2))$$
$$-(a_2-a_1)(XK_x+YK_y)))$$

$$\langle d(x^2-y^2)|\cos|d_{(3_z{}^2-r^2)}\rangle = C_{14}DTEW^3(\cos(\tfrac{1}{4}W(\tfrac{1}{4}(K_x{}^2-K_y{}^2)$$
$$-a_2^2(X^2-Y^2)(2K_z{}^2-K_x{}^2-K_y{}^2)$$
$$+W(2Z^2-X^2-Y^2)(a_1^2a_2^2(X^2-Y^2$$
$$-\tfrac{1}{4}a_1^2(K_x{}^2-K_y{}^2))$$
$$+2a_1a_2(X^2-Y_2)+\tfrac{1}{2}(K_x{}^2-K_y{}^2)$$
$$+L(2ZK_z-XK_x-YK_y)(XK_x-YK_y))$$
$$+\sin(a_2W(XK_x-YK_y)(\tfrac{1}{4}(2K_z{}^2-K_x{}^2$$
$$-K_y{}^2)-a_1^2(2Z^2-X^2-Y^2))$$
$$+(a_2L(X^2-Y^2)-\tfrac{1}{4}a_1W(K_x{}^2-K_y{}^2))$$
$$(2ZK_z-XK_x-YK_y)+(a_2-a_1)(XK_x-YK_y)))$$

$$\langle d_{(3_z{}^2-r^2)}|\cos|d(3_z{}^2-r^2)\rangle = C_{15}DTEW^3(\cos(a_1a_2L(2Z^2-X^2-Y^2)^2$$
$$-2a_1a_2(4Z^2+X^2+Y^2)+3/W$$
$$-\tfrac{1}{4}W(a_1^2+a_2^2)(2Z^2-X^2-Y^2)(2K_z{}^2-K_x{}^2$$
$$-K_y{}^2)+L(2ZK_z-XK_x-YK_y)^2+W(2K_z{}^2$$
$$-K_x{}^2-K_y{}^2)^2\ /16-\tfrac{1}{2}(4K_z{}^2+K_x{}^2+K_y{}^2))$$
$$+(a_2-a_1)\sin((2ZK_z-XK_x-YK_y)$$
$$(L(2Z^2-X^2-Y^2)+\tfrac{1}{4}W(2K_z{}^2-K_x{}^2-K_y{}^2))$$
$$-(4ZK_z+XK_x+YK_y)))$$

```
C          THIS PGM CALCULATES THE D-D 3-CENTERED INTEGRALS AND
C      2-CENTERED INTEGRALS NECESSARY IN THE BAND PGM
       IMPLICIT REAL*8(A-F,H,O-Z)
       DIMENSION GS15(15),RSQU(15),RSQ(15),SOLUP(15),SOLDN(15),SUMUP(15),
      1SUMDN(15),GRKUP(1000),GRKDN(1000),SEXUP(25,25),SEXDN(25,25),
      2SR2(25,25)
       DIMENSION S(20),EKS(20)
       DIMENSION EK(15),ALD(5),CD(5),SS(20),SUM(20),SUM1(20),GER(40)
       DIMENSION SOLD(20),SOL1(20),CD1(5)
       DIMENSION GVK(1000),GRK(1000),GB(1000),GC(1000),GD(1000),IOU(1000)
       DIMENSION SPOT(25,25),SEXC(25,25),SKE(25,25),SOVLP(25,25)
       COMMON CON1,CON2,CON3,CON4,CON5,CON6,S,RSQU,EKS,RAB,ALPHA1,
      1ALPHA2,RS,AI,AJ,AK,AX,AY,AZ,BX,BY,BZ,CX,CY,CZ,ALAMDA,ADELTA,
      2AZETA,U,PI,N
       PI=3.141592653589793
C      READ VECTOR COEFFICIENTS FOR D-WAVEFUNCTION
       READ(5,4000)(CD1(I),I=1,5)
 4000  FORMAT(5F10.6)
C      READ ALPHAMERIC DEFINING PARAMETERS
       READ(5,6)(GER(I),I=1,30)
    6  FORMAT(26A3/4A3)
C      READ NUMBER OF RECIPROCAL LATTICE VECTORS
       READ(5,101)JJJJ
  101  FORMAT(I5)
C      READ DIRECT LATTICE VECTORS/2, IE, A/2
       READ(5,641)QA
  641  FORMAT(F9.6)
C      READ POSITIVE PERMUTATIONS OF RECIPROCAL LATTICE VECTORS
       DO 401 J=1,JJJJ
       READ(8) GVK(J),GRK(J),GRKUP(J),GRKDN(J),GB(J),GC(J),GD(J),IOU(J)
  401  CONTINUE
C      READ ORBITAL EXPONENTS, ALD(J), AND VECTOR COEFFICIENTS, CD(J),
C           AND NORMALIZE THE CD(J)
       DO 10 J=1,5
```

```
      READ(5,3)ALD(J),CD(J)
      AAA=8.D0*ALD(J)/ DSQRT(15.D0)*(8.D0*ALD(J)**3/PI)**.25
   10 CD(J)=CD(J)*AAA
    3 FORMAT(F8.6,E16.8)
      NRC=0
C       READ X,Y,Z COMPONENTS OF 3 CENTERS , FOR EXAMPLE,  1 1 0 0 0 0 0 0 0
C       INDICATES FIRST NEIGHBOR SEPARATION,  WITH SECOND WAVEFUNCTION
C       SITUATED AT THE ORIGIN AND THE POTENTIAL SITUATED ON THE ORIGIN
   60 READ(5,4)IAX,IAY,IAZ,IBX,IBY,IBZ,ICX,ICY,ICZ
    4 FORMAT(9I5)
      AX=IAX*QA
      AY=IAY*QA
      AZ=IAZ*QA
      BX=IBX*QA
      BY=IBY*QA
      BZ=IBZ*QA
      CX=ICX*QA
      CY=ICY*QA
      CZ=ICZ*QA
      NRC=NRC+1
      DO 398 J=1,15
      RSQ(J)=0.0
      SOLUP(J)=0.0
      SOLDN(J)=0.0
      SS(J)=0.0
      EK(J)=0.0
      SOL1(J)=0.0
  398 SOLD(J)=0.0
      CON1=BX-AX
      CON2=BY-AY
      CON3=BZ-AZ
      CON4=CON1**2
      CON5=CON2**2
      CON6=CON3**2
C     DO LOOPS OVER S-D ORBITALS PERFORMS THE INTEGRAL OF
```

```
C            ( ORBITAL(I) * H * ORBITAL (J) D3R )
      DO 40 L=1,5
      DO 40 K=1,5
      CDC=CD(L)*CD(K)
      ALPHA1=ALD(L)
      ALPHA2=ALD(K)
      RAB=DSQRT(CON4+CON5+CON6)
      DO 100 J=1,15
      SS(J)=0.0
      SUM1(J)=0.0
      SUMUP(J)=0.0
      SUMDN(J)=0.0
  100 SUM(J)=0.0
C      DEFINE APPROPRIATE PARAMETERS FROM LAFON AND LIN
      ALAMDA=ALPHA1*ALPHA2/(ALPHA1+ALPHA2)
      ADELTA=PI/(ALPHA1+ALPHA2)
      ADELT=DSQRT(ADELTA)
      ADELTA=ADELTA*ADELT
      EXPA=ALAMDA*RAB**2
      IF(EXPA.GT.75.0)AZETA=0.0
      IF(EXPA.LE.75.0)AZETA=DEXP(-EXPA)
      U=ALPHA1/(ALPHA1+ALPHA2)
C     PERFORM SUM OVER RECIPROCAL LATTICE VECTORS
      DO 500 J=1,JJJJ
      N=IOU(J)
      AI=PI/QA*GB(J)
      AJ=PI/QA*GC(J)
      AK=PI/QA*GD(J)
      SK=DSQRT(AI*AI+AJ*AJ+AK*AK)
      RS=SK*SK
C      D3INT CALCULATES ACTUAL 3-CENTER INTEGRAL
      CALL D3INT
      DO 146 N=1,15
      IF(J.NE.1)GO TO 145
      SS(N)=SS(N)+S(N)*CDC
```

```
  145 SUM1(N)=SUM1(N)+GRK(J)*S(N)
      SUMUP(N)=SUMUP(N)+GRKUP(J)*S(N)
      SUMDN(N)=SUMDN(N)+GRKDN(J)*S(N)
      SUM(N)=SUM(N)+GVK(J)*S(N)
  146 CONTINUE
  500 CONTINUE
      CALL R2
      CALL KINE
C     RSQ IS R SQUARED INTEGRALS, SOLUP IS UP-SPIN EXCHANGE,SOLDN IS
C      DOWN-SPIN EXCHANGE, EK IS KINETIC ENERGY, SOL1 IS PARAMAGNETIC
C      EXCHANGE, AND SOLD IS THE COULOMB POTENTIAL INTEGRAL.
      DO 408 J=1,15
      RSQ(J)=RSQ(J)+RSQU(J)*CDC
      SOLUP(J)=SOLUP(J)+SUMUP(J)*CDC
      SOLDN(J)=SOLDN(J)+SUMDN(J)*CDC
      EK(J)=EK(J)+EKS(J)*CDC
      SOL1(J)=SOL1(J)+SUM1(J)*CDC
  408 SOLD(J)=SOLD(J)+SUM(J)*CDC
      CDD1=CD1(L)*CD1(K)
      N100=2
C      SETS UP 25 X 25 MATRIX FOR INTEGRALS NEEDED,IE, INDIVIDUAL ORBITALS
C      FROM 15 INDEPENDENT INTEGRALS
      DO 8071 J=1,15
      GO TO (8051,8052,8053,8054,8055,8056,8057,8058,8059,8060,8061,
     18062,8063,8064,8065),J
 8070 SPOT(L25+L,K25+K)=SUM(J)*CDC/CDD1
      SR2(L25+L,K25+K)=RSQU(J)*CDC/CDD1
      SEXUP(L25+L,K25+K)=SUMUP(J)*CDC/CDD1
      SEXDN(L25+L,K25+K)=SUMDN(J)*CDC/CDD1
      SEXC(L25+L,K25+K)=SUM1(J)*CDC/CDD1
      SKE(L25+L,K25+K)=EKS(J)*CDC/CDD1
      SOVLP(L25+L,K25+K)=SS(J)/CDD1
 8071 CONTINUE
   40 CONTINUE
      GO TO 9090
```

```
C       PARAMETERS BELOW ORDER THE INDEPENDENT INTEGRALS ACCORDING TO
C       25 X 25 MATRIX, IN ORDER D1 TO D5 FOR XY, D1 TO D5 FOR YZ,
C       D1 TO D5 FOR XZ, D1 TO D5 FOR (X**2-Y**2), AND D1 TO D5 FOR
C         (3Z**2-R**2)
 8051 L25=20
      K25=20
      GO TO (7070,8070,9070),N100
 8052 L25=0
      K25=0
      GO TO (7070,8070,9070),N100
 8053 L25=10
      K25=10
      GO TO (7070,8070,9070),N100
 8054 L25=5
      K25=5
      GO TO (7070,8070,9070),N100
 8055 L25=15
      K25=15
      GO TO (7070,8070,9070),N100
 8056 L25=5
      K25=10
      GO TO (7070,8070,9070),N100
 8057 L25=15
      K25=20
      GO TO (7070,8070,9070),N100
 8058 L25=0
      K25=10
      GO TO (7070,8070,9070),N100
 8059 L25=0
      K25=15
      GO TO (7070,8070,9070),N100
 8060 L25=5
      K25=20
      GO TO (7070,8070,9070),N100
 8061 L25=10
```

```
      K25=20
      GO TO (7070,8070,9070),N100
 8062 L25=0
      K25=20
      GO TO (7070,8070,9070),N100
 8063 L25=0
      K25=5
      GO TO (7070,8070,9070),N100
 8064 L25=5
      K25=15
      GO TO (7070,8070,9070),N100
 8065 L25=10
      K25=15
      GO TO (7070,8070,9070),N100
 9090 CONTINUE
      DO 8075 J=1,25
      DO 8075 K1=1,J
      SR2(J,K1)=SR2(K1,J)
      SEXUP(J,K1)=SEXUP(K1,J)
      SEXDN(J,K1)=SEXDN(K1,J)
      SPOT(J,K1)=SPOT(K1,J)
      SKE(J,K1)=SKE(K1,J)
      SEXC(J,K1)=SEXC(K1,J)
 8075 SOVLP(J,K1)=SOVLP(K1,J)
      WRITE(6,2) AX,AY,AZ
      WRITE(6,2) BX,BY,BZ
      WRITE(6,2) CX,CY,CZ
    2 FORMAT(3F10.6)
C      RESUM TO RECLAIM THE TOTAL D WAVEFUNCTION INTEGRALS
      DO 8002 J=1,15
      RSQ(J)=0.0
      SOLUP(J)=0.0
      SOLDN(J)=0.0
      SOLO(J)=0.0
      SOL1(J)=0.0
```

```
      EK(J)=0.0
 8002 SS(J)=0.0
      N1CO=1
      DO 7071 J=1,15
      GO TO (8051,8052,8053,8054,8055,8056,8057,8058,8059,8060,8061,
     18062,8063,8064,8065),J
 7070 L20=L25+1
      K20=K25+1
      L26=L25+5
      K26=K25+5
      DO 7080 L=L20,L26
      DO 7080 K=K20,K26
      CDD1=CD1(L-L25)*CD1(K-K25)
      RSQ(J)=RSQ(J)+SR2(L,K)*CDD1
      SOLUP(J)=SOLUP(J)+SEXUP(L,K)*CDD1
      SOLDN(J)=SOLDN(J)+SEXDN(L,K)*CDD1
      SOLD(J)=SOLD(J)+SPOT(L,K)*CDD1
      SOL1(J)=SOL1(J)+SEXC(L,K)*CDD1
      EK(J)=EK(J)+SKE(L,K)*CDD1
 7080 SS(J)=SS(J)+SOVLP(L,K)*CDD1
 7071 CONTINUE
      WRITE(6,8005)
 8005 FORMAT(1X,'FOLLOWING IS TO CHECK MATRIX ELEMENTS')
      DO 8003 J=1,15
      JJ=2*J-1
      WRITE(6,8)GER(JJ),GER(JJ+1)
 8003 WRITE(6,1)SOLD(J),SOL1(J),SOLUP(J),SOLDN(J),EK(J),SS(J),RSQ(J)
    1 FORMAT(1X,'P=',E16.8,'X=',E15.8,'U=',E15.8,'DN=',E16.8,'K=',
     1E16.8,'UV=',E16.8,'R=',E16.8)
    8 FORMAT(2A3)
C       WRITE OUT INTEGRALS FOR GIVEN VALUE OF DIRECT LATTICE VECTOR,
C       WITH IDENTIFYING INTEGERS FOR NEAREST NEIGHBOUR, AND POSITION IN MATRIX
      DO 8010 I2=1,25
      DO 8010 I3=1,I2
      G1=SPOT(I2,I3)
```

```
      G2=SEXC(I2,I3)
      G3=SEXUP(I2,I3)
      G4=SEXDN(I2,I3)
      G5=SKE(I2,I3)
      G6=SOVLP(I2,I3)
      G7=SR2(I2,I3)
 8010 WRITE(12)NRC,I2,I3,G1,G2,G3,G4,G5,G6,G7
      GO TO 60
 7070 CONTINUE
    8 FORMAT(2A3)
 9070 WRITE(6,9999)
 9999 FORMAT(1X,'REACHED 9070 ILLEGALLY')
      END
      SUBROUTINE  D3INT
C       THIS SUBROUTINE PERFORMS 3-CENTER INTEGRALS
      IMPLICIT REAL*8(A-F,H,O-Z)
      DIMENSION S(20),EKS(20),RSQU(15)
      COMMON CON1,CON2,CON3,CON4,CON5,CON6,S,RSQU,EKS,RAB,ALPHA1,
     1ALPHA2,RS,AI,AJ,AK,AX,AY,AZ,BX,BY,BZ,CX,CY,CZ,ALAMDA,ADELTA,
     2AZETA,U,PI,N
      DO 150 J=1,15
  150 S(J)=0.0
      IF(AZETA.EQ.0.0) GO TO 50
C       CON IS A MULTIPLICATIVE CONSTANT DEPENDENT ON POSITIVE
C       PERMUTATIONS OF THE RECIPROCAL LATTICE VECTORS WHICH WERE READ IN.
C       N=4 FOR (000), N=3 FOR (A,0,0) TYPE, N=2 FOR (A,A,0) OR (A,B,0) TYPE,
C       AND N=1 FOR ALL OTHER TYPES.
      GO TO (10,11,12,15),N
   15 CON=1.D0
      GO TO 206
   10 CON=8.D0
      GO TO 206
   11 CON=4.D0
      GO TO 206
   12 CON=2.D0
```

```
  206 CONTINUE
      EXPB=RS/(4.D0*(ALPHA1+ALPHA2))
      IF(EXPB.GT.75.0)GO TO 5
      ADEL=DEXP(-EXPB)
      GO TO 6
    5 ADEL=0.0
      GO TO 50
    6 CONTINUE
C       DEFINES COS (K. RCD) PARAMETERS
      DX=AX*U+BX*(1.D0-U)
      DY=AY*U+BY*(1.D0-U)
      DZ=AZ*U+BZ*(1.D0-U)
      RCDX=DX-CX
      RCDY=DY-CY
      RCDZ=DZ-CZ
      S1=DSIN(AI*RCDX)
      S2=DSIN(AJ*RCDY)
      S3=DSIN(AK*RCDZ)
      C1=DCOS(AI*RCDX)
      C2=DCOS(AJ*RCDY)
      C3=DCOS(AK*RCDZ)
      SA=S1*C2*C3*CON
      SB=C1*S2*C3*CON
      SC=C1*C2*S3*CON
      SD=-S1*S2*S3*CON
      CD=C1*C2*C3*CON
      CC=-S1*S2*C3*CON
      CB=-S1*C2*S3*CON
      CA=-C1*S2*S3*CON
      A0=1.19366207
      A1=0.89524655/9.D0
      A2=0.29841552
      A3=0.51687084/3.D0
      A4=0.59683104
      A5=1.03374168/3.D0
```

```
      A6=ALAMDA**3*ADELTA*ADEL*AZETA/(4.D0*ALPHA1**2*ALPHA2**2)
      A7=A6/ALAMDA
      A8=0.5D0/(ALPHA1*ALPHA2)
      A9=0.25D0/(ALPHA1*ALPHA2**2)
      A10=(2.D0*U-1.D0)/ALAMDA
      A11=0.5D0/(ALAMDA*ALPHA2)
      A12=(1.D0-U)*(2.D0*U-1.D0)
      A13=2.D0*ALAMDA
      A14=1.D0/ALAMDA
      A15=(2.D0*U-1.D0)
      A16=(1.D0-U)
      A17=1.D0/(2.D0*ALPHA2**2)
      A18=1.D0/(2.D0*ALPHA1**2)
      A19=AI*AI-AJ*AJ
      A20=CON4-CON5
C     XY-XY   INTEGRAL
      S(2)=A6*A0*(((1.D0-A13*CON5)*(A14-2.D0*CON4-AI*AI*A8)+A16*AJ*AJ*
     1(AI*AI*A9+CON4/ALPHA2-A11))*C0-CON1*CON2  *AI*AJ*CC*A15*A15/ALAMDA
     2-A15*A14*CON1*AI*SA*(A13*CON5-1.D0)-A13*CON2*AJ*SB*(AI*AI*A9+CON4/
     3ALPHA2-A11)-CON2*AJ*SB*A15*(A14-2.D0*CON4-AI*AI*A8)-A12*CON1*AI*SA
     4*AJ*AJ*A11)
C       XY-XZ   INTEGRAL
      S( 8)=A6*A0*(A13*CON1*AI*(A8  *CON2*AK*CB-CON3*AJ*CC*A17)
     1-(1.D0-A13*CON4)*(2.D0*CON2*CON3*C0+A8*AJ*AK*CA)+AI*AI*
     2A16*(CON2*CON3/ALPHA2*C0+AJ*AK*A9*CA)+CON1*AI*A16*(AJ*CC*CON3/
     3ALPHA2-AK*CB*CON2/ALPHA1)+AI*AI*A16*(AK*SC*CON2*A8-AJ*SB*CON3*A17)
     4+AI*A16*CON1  *(2.D0*CON2*CON3*SA+AJ*AK*SD*A8)-A13*CON1*(AI*SA
     5*CON2*CON3/ALPHA2+AI*AJ*AK*SD*A9)+(1.D0-A13*CON4)*(CON3*AJ*SB/
     6ALPHA2-AK*SC*CON2/ALPHA1))
C       XY-YZ  INTEGRAL
      S( 13)=A6*A0*(A13*CON2*(AJ*AK*CA*CON1*A8-AI*AJ*CC*A17*CON3)-(1.D0-
     1A13*CON5)*(2.D0*CON1*CON3*C0+AI*AK*CB*A8)+AJ*AJ*A16*(AI*AK*CB*A9
     2+CON1*CON3/ALPHA2*C0)+CON2*AJ*A16*(AI*CC*CON3/ALPHA2-AK*CA*CON1/
     3ALPHA1)+AJ*A16*(AJ*AK*SC*CON1*A8-AJ*AI*SA*CON3*A17)+CON2*AJ*A16*
     4(2.D0*CON1*CON3*SB+AI*AK*SD*A8)-A13*CON2*(AI*AJ*AK*SD*A9+AJ*SB*
```

```
     5CON1*CON3/ALPHA2)+(1.DC-A13*CUN5)*(AI*SA*CON3/ALPHA2-AK*SC*CON1/
     6ALPHA1))
C      XZ-XZ  INTEGRAL
      S( 3)=A6*A0*((((1.DC-A13*CON6)*(A14-2.D0*CON4-AI*AI*A8)+AK*AK*A16*
     1(AI*AI*A9+CON4/ALPHA2-A11))*CO-AI*AK*CB*A14*CON1*CON3*A15*A15
     2-CON1*AI*SA*A10*(A13*CUN6-1.DC)-A13*CON3*AK*SC*(AI*AI*A9+CON4/
     3ALPHA2-A11)-CON3*AK*SC*A16*(A14-2.D0*CON4-AI*AI*A8)-CON1*AI*SA*
     4AK*AK*A11*A12)
C      YZ-YZ   INTEGRAL
      S( 4)=A6*A0*((((1.D0-A13*CON6)*(A14-2.D0*CON5-AJ*AJ*AB)+AK*A16*
     1AK*(AJ*AJ*A9+CON5/ALPHA2-A11))*CO-AK*AJ*CA*A14*CON2*CON3*A15*A15
     2-CON2*AJ*SB*A15*A14*(A13*CON6-1.D0)-A13*CON3*(AJ*AJ*AK*SC*A9+AK*
     3CON5/ALPHA2*SC-AK*SC*A11)-CON3*AK*SC*A16*(A14-2.D0*CON5-AJ*AJ*
     4A8)-CON2*AK*AK*AJ*SB*A11*A12)
C     YZ-XZ  INTEGRAL
      S( 6)=A6*AC*(A13*CON3*(CON2*AI*AK*CB*A8-CON1*AJ*AK*A17*CA)-(1.D0-
     1A13*CON6)*(2.D0*CON1*CON2*CO+AJ*AI*CC*A8)+AK*AK*A16*(CON1*CON2/
     2ALPHA2*CO+AI*AJ*CC*A9)+CON3*AK*A16*(CON1*AJ*CA/ALPHA2-CON2*AI*CB/
     3ALPHA1)+AK*AK*A16*(AI*CON2*A8*SA-AJ*SB*CON1*A17)+AK*A16*CON3*
     4(2.D0*CON1*CON2*SC+AI*AJ*SD*A8)-A13*CON3*(AK*SC*CON1*CON2/ALPHA2
     5+AI*AJ*AK*SD*A9)+(1.DC-A13*CON6)*(CON1*AJ*SB/ALPHA2-AI*SA*CON2/
     6ALPHA1))
      X20=(3.D0*U-1.D0)
      X21=(3.D0*U-2.D0)
C       XY-(X**2-Y**2)  INTEGRAL
      S( 9)=A6*A4*((X20*A19/ALPHA1       *CON1*CON2+2.DC*A13*A20*CON1*CON2
     1)*CO+AI*AJ*CC*(-X21*A20/ALPHA2+A19*A16*A9)-
     2X21*2.D0*CON1*CON2   *(AI*SA*CON1-AJ*SB*CON2)+2.D0/ALAMDA*(AJ*SB*
     3CON1-AI*SA*CON2)-X20     *A8         *AI*AJ*(AI*SB*CON1-AJ*SA*CON2)
     4+ALAMDA*A8/ALPHA1*(CON2*AI**3*SA-CON1*AJ**3*SB)-A13/ALPHA2*(AJ*SB
     5*CON4*CON1-AI*SA*CON5*CON2))
      DC=0.25D0/(ALPHA1+ALPHA2)**2
      D1=AI*AJ*A17*0.5DC
      D2=1.DC-A13*CON6
      D3=ADELTA*ADEL*AZETA*A18*0.5DC
```

```
      D4=CON1*CON2
      RA=RA3**2
      D5=AI*AJ
      D8=CON2*CON3
      D7=AJ*AK/(4.D0*ALPHA2**2)
      B1=2.D0*D7*(1.D0-A13*CON4)*CA+D7*(A16*AI*AI/ALPHA1)*CA
     1+2.D0*A13*CON4*D8*CO+AI*CON1*(CON2*AK*CB+CON3*AJ*CC)*(A13*A8+A16/
     2ALPHA2)+D8*(-AI*AI*A16/ALPHA1-AJ*AJ*A13*A8+4.D0*(1.D0-ALAMDA*
     3CON5)-AJ*AJ*A15/ALPHA1)*CO-AJ*AK*A10/(2.D0*ALPHA2)*(1.D0-A13*CON5)
     4*CA-AJ*A16*(AJ*AJ*AK*CA*A9-AK*CA*A11)-AJ*AK*CA*A16*CON5/ALPHA2
      B2=(CON2*AK*SC+CON3*AJ*SB)*(AI*AI*A16*A8+(1.D0-A13*CON4)/ALPHA2)
     1-2.D0*CON1*AI*(D7*SD-D8*SA)*(A16+ALAMDA/ALPHA1)-AJ*A16*CON3*SB*
     2(AJ*AJ*A8-1.D0/ALAMDA)-2.DC*A16*CON3*CON5*AJ*SB+A15*A8*CON2*AJ*AJ
     3*AK*SC+A13*CON2*(A9*AJ*AJ*AK*SC-AK*SC*A11)-2.D0*AK*SC*CON2/ALPHA2
     4*(1.D0-ALAMDA*CON5)-A15*A14*CON3*AJ*SB*(1.D0-A13*CON5)
C       YZ-(X**2-Y**2)  INTEGRAL
      S(14)=A6*A4*(B1+B2)
      D9=CON1*CON3
      D10=1.D0-2.D0*ALAMDA*CON4
      D11=1.D0-ALAMDA*CON4
      D12=1.D0-2.D0*ALAMDA*CON5
      D13=1.D0-ALAMDA*CON5
      B1=A13*D9*CO*(AI*AI*A8-A14)-4.D0*D9*(1.D0-ALAMDA*CON4)*CO+AI*AK*CB
     1*A11*A15*D10+AI*AK*CB*A16*(A9*AI*AI-A11)+AI*AK*CB*A16*CON4/ALPHA2
     2+AI*AI*A15/ALPHA1*D9*CO-2.D0*ALPHA2*A14*(D9*CO-AI*AK*CB*A17*0.5D0)
      B2=2.D0*D12*(AI*AK*CB*A17*0.5D0-D9*CO)+AJ*CON2*(CON3*AI*CC+CON1*
     1AK*CA)*(A13*A8+A16/ALPHA2)+(AI*AK*CB/(4.D0*ALPHA2**2)-D9*CO)
     2*(AJ*AJ*A16/ALPHA1+2.D0*ALPHA2*A14)
      B3=AI*SA*(A16*CON3*(AI*AI*A8-A14)+2.D0*A16*D9*CON1)+AK*SC*(-AI*AI
     1*A15*CON1*A8+A13*CON1*(A11-AI*AI*A9)+2.D0*CON1/ALPHA2*D11)
     2+D10*CON3*AI*SA*A15*A14+A14*(CON3*AI*SA+CON1*AK*SC)
      B4=AJ*AJ*A16*A8*(CON3*AI*SA+CON1*AK*SC)-CON2*AJ*(AI*AK*SD*A17
     1*0.5D0-D9*SB)*(2.D0*A16+A13/ALPHA1)+(CON3*AI*SA+CON1*AK*SC)*(D12/
     2ALPHA2+A14)
C       XZ-(X**2-Y**2)  INTEGRAL
```

```
      S(15)=A4*A6*(B1+B3-B2-B4)
      Z1=CON4+CON5-2.DC*CON6
      Z2=AI*AI+AJ*AJ-2.DC*AK*AK
      Z3=CON1*AI*SA+CON2*AJ*SB-2.D0*CON3*AK*SC
C       XZ-(3Z**2-R**2) INTEGRAL
      S(11)=A6*A5*(-4.D0*D9*CO-2.D0*AI*AK*CB*A8+Z1*(AI*AK*CB*A16/ALPHA1
     1-2.D0*A13*D9*CO)+Z2*(U*D9*CO/ALPHA2-A15*AI*AK*A9*CB)-2.D0*A16/
     2ALPHA2*(CON1*AK*(AI*CB*CON1+CON2*AJ*CA-2.D0*AK*CO*CON3)+
     3CON3*AI*(CON1*AI*CO+CON2*AJ*CC-2.D0*CON3*AK*CB))+4.D0*(CON1*AK*
     4SC/ALPHA2-CON3*AI*SA/ALPHA1)+U*A8*Z2*(CON3*AI*SA+CON1*AK*SC)
     5-2.D0*A16*Z1*(CON3*AI*SA+CON1*AK*SC)+4.D0*U*D9*Z3-A16*2.D0*A8
     6*AI*AK*(CON1*AI*SC+CON2*AJ*SD-2.D0*CON3*AK*SA)+2.D0*(CON1*AK*SC/
     7ALPHA1-CON3*AI*SA/ALPHA2))
C       XY-(3Z**2-R**2) INTEGRAL
      S(12)=A6*A5*(8.DC*D4*CO+4.D0*A8*D5*CC+Z1*(AI*AJ*A16*CC/ALPHA1-
     12.D0*A13*D4*CO)-2.D0*A16/ALPHA2*(CON1*AJ*(CON1*AI*CC+CON2*AJ*CO
     2-2.D0*CON3*AK*CA)+CON2*AI*(CON1*AI*CO+CON2*AJ*CC-2.D0*CON3*AK*CB))
     3+Z2*(U*D4/ALPHA2*CO-AI*AJ*A9*CC*A16)+(CON2*AI*SA+CON1*AJ*SB)*
     4(2.D0/ALPHA1-2.D0/ALPHA2-2.D0*A16*Z1)
     $+Z2*U*A8*(CON1*AJ*SB+CON2*AI*SA)
     5+4.D0*U*D4*Z3-AI*AJ*A16*2.D0*A8*(CON1*AI*SB+CON2*AJ*SA-2.D0*
     6CON3*AK*SD))
C       YZ-(3Z**2-R**2) INTEGRAL
      S(10)=A6*A5*(-4.DC*D8*CO-2.D0*AJ*AK*CA*A8+Z1*(AJ*AK*CA*A16/ALPHA1
     1-2.DC*A13*D8*CO)+Z2*(U*D8*CO/ALPHA2-A15*AJ*AK*A9*CA)-2.D0*A16/
     2ALPHA2*(CON2*AK*(AI*CB*CON1+CON2*AJ*CA-2.D0*AK*CO*CON3)+
     3CON3*AJ*(CON1*AI*CC+CON2*AJ*CO-2.D0*CON3*AK*CA))+4.D0*(CON2*AK*
     4SC/ALPHA2-CON3*AJ*SB/ALPHA1)+U*A8*Z2*(CON3*AJ*SB+CON2*AK*SC)
     5-2.D0*A16*Z1*(CON3*AJ*SB+CON2*AK*SC)+4.D0*U*D8*Z3-A16*2.D0*A8
     6*AJ*AK*(CON1*AI*SD+CON2*AJ*SC-2.D0*CON3*AK*SB)+2.D0*(CON2*AK*SC/
     7ALPHA1-CON3*AJ*SB/ALPHA2))
      B1=(4.DC-4.DC*A13*(CON4+CON5)+A13*A13*A20**2-(CON4-CON5)*A19*
     1(U*U+A16*A16)+A8*A8*ALAMDA*ALAMDA*A19**2-2.D0*A13*A8*(AI*AI+AJ*AJ)
     2)*CO+4.D0*U*A16*((CON4*AI*AI+CON5*AJ*AJ)*CO-2.D0*D4*D5*CC)
      B2=4.DC*A15*(CON1*AI*SA+CON2*AJ*SB)+(CON1*AI*SA-CON2*AJ*SB)
```

```
     1*(A19*(A16*A16/ALPHA2-U*U/ALPHA1)-A15*4.D0*ALAMDA*A20)
C       (X**2-Y**2)-(X**2-Y**2) INTEGRAL
      S(5)=A7*A2*(B1+B2)
      D14=AI*AI+AJ*AJ-2.D0*AK*AK
      D15=CON4+CON5-2.D0*CON6
      D31=CON4+CON5-CON6
      B1=(D15*(A16/ALPHA1*A19-2.D0*A13*A20)+D14*(U/ALPHA2*A20 -A15*A9*
     1A19)+4.D0*A8*A19+8.D0*A20)*CD-4.D0*U/ALPHA1*(CON1*AI*(CON1*AI*CD
     2+CON2*AJ*CC-2.D0*CON3*AK*CB)-CON2*AJ*(CON1*AI*CC+CON2*AJ*CD-2.D0*
     3CON3*AK*CA))
      B2=(CON1*AI*SA-CON2*AJ*SB)*(2.D0*U*A8*D14-4.D0*A15*A14
     $-4.D0*A16*D15)
     1-Z3*A16*2.D0*A8*A19+4.D0*U*A20*Z3
C       (X**2-Y**2)-(3Z**2-R**2) INTEGRAL
      S(7)=A6*A3*(B1+B2)
      B1=(4.D0-8.D0*A13*CON6+(A13*D2+AK*AK*A16*A16)*D15+D14*(U*J*CON6-
     1U*0.5D0/ALPHA2-AK*AK*A16*A15*A17*0.5D0)-4.D0*U/ALPHA1*AK*AK)*CD
     2-4.D0*U*A16*CON3*AK*(CON1*AI*CB+CON2*AJ*CA-2.D0*CON3*AK*CD)
      B2=-D15*2.D0*A13*A16*CON3*AK*SC+(2.D0*A13*U*CON6-2.D0*U-U*A16/
     1ALPHA1*AK*AK)*Z3+D14*U*A16/ALPHA2*CON3*AK*SC+8.D0*A15*CON3*AK*SC
      Z10=CON4+CON5
      Z11=AI*AI+AJ*AJ
      B3=((2.D0*A13*Z10-4.D0-A16/ALPHA1*Z11)*D15+D14*(A17*2.D0-U/ALPHA2
     1*Z10+A16*A9*Z11)-4.D0*A8*Z11+4.D0*A14-8.D0*Z10)*CD+4.D0*U/ALPHA1*
     2(CON1*AI*(CON1*AI*CD+CON2*AJ*CC-2.D0*CON3*AK*CB)+CON2*AJ*
     3(CON1*AI*CC+CON2*AJ*CD-2.D0*CON3*AK*CA))
      B4=(CON1*AI*SA+CON2*AJ*SB)*(4.D0*A16*D15-2.D0*U*A8*D14+4.D0*A15*
     1A14)+Z3*(4.D0/ALPHA2+2.D0*A16*A8*Z11-4.D0*U*Z10)
C       (3Z**2-R**2)-(3Z**2-R**2)   INTEGRAL
      S(1)=A1*A6*(2.D0/ALAMDA*(B1+B2)+(B3+B4))
   50 CONTINUE
      RETURN
      END
      SUBROUTINE KINE
C       THIS SUBROUTINE CALCULATES THE KINETIC ENERGY INTEGRALS
```

```
      IMPLICIT REAL*8(A-F,H,O-Z)
      DIMENSION S(20),EKS(20),RSQU(15)
      COMMON CON1,CON2,CON3,CON4,CON5,CON6,S,RSQU,EKS,RAB,ALPHA1,
     1ALPHA2,RS,AI,AJ,AK,AX,AY,AZ,BX,BY,BZ,CX,CY,CZ,ALAMDA,ADELTA,
     2AZETA,U,PI,N
      DO 150 J=1,15
  150 EKS(J)=0.0
      IF(AZETA.EQ.0.0)GO TO 50
      A1=1.19366207*2.D0
      A2=1.03374168*2.D0/3.D0
      A3=0.59683104*2.D0
      A4=0.51687084*2.D0/3.D0
      A5=0.29841552*2.D0
      A6=0.89524655*2.D0/9.D0
      A7=ALAMDA**3*0.5D0*ADELTA   *AZETA/(ALPHA1**2*ALPHA2**2)
      A8=2.D0*A7*ALAMDA
      A9=A8*ALAMDA
      A10=CON4+CON5-2.D0*CON6
      A11=9.D0-2.D0*ALAMDA*RAB**2
      A12=ALAMDA*(2.D0*ALAMDA*RAB**2-11.D0)
      RA=RAB**2
      A13=ALAMDA**2
C       (3Z**2-R**2)-(3Z**2-R**2)   INTEGRAL
      EKS(1)=2.D0*A7*A6*(21.D0-6.D0*ALAMDA*RA-2.D0*(9.D0*ALAMDA-2.D0*RA
     1*ALAMDA**2)*(CON4+CON5+4.D0*CON6)+A10*A10*A13*(11.D0-2.D0*ALAMDA
     2*RA))
C     XY-XY   INTEGRAL
      EKS(2)=A7*A1*((3.5D0-9.D0*ALAMDA*CON5)*(1.D0-2.D0*CON4*ALAMDA)
     1+(2.D0*A13*CON5-ALAMDA)*(2.D0*CON4+RA-2.D0*ALAMDA*CON4*RA))
C       XZ-XZ INTEGRAL
      EKS(3)=A7*A1*((3.5D0-9.D0*ALAMDA*CON6)*(1.D0-2.D0*CON4*ALAMDA)
     1+(2.D0*A13*CON6-ALAMDA)*(2.D0*CON4+RA-2.D0*ALAMDA*CON4*RA))
C       YZ-YZ   INTEGRAL
      EKS(4)=A7*A1*((3.5D0-9.D0*ALAMDA*CON5)*(1.D0-2.D0*ALAMDA*CON6)
     1+(2.D0*A13*CON5-ALAMDA)*(2.D0*CON6+RA-2.D0*ALAMDA*CON6*RA))
```

```
C       (X**2-Y**2)-(X**2-Y**2) INTEGRAL
      EKS(5)=A5*A7*2.D0*(7.D0+(CON4+CON5)*( 4.D0*A13*RA-18.D0*ALAMDA)+
     1CON4*CON5*( 4.D0*A13*ALAMDA*RA-22.D0*A13)+(CON4**2+CON5**2)*(
     211.D0*A13-2.D0*A13*ALAMDA*RA)-2.D0*ALAMDA*RA)
C      YZ-XZ INTEGRAL
      EKS(6)=A8*A1*CON1*CON2*(-4.5D0+ALAMDA*(11.D0*CON6
     1+RA)-2.D0*A13*CON6*RA)
C       (X**2-Y**2)-(3Z**2-R**2) INTEGRAL
      EKS(7)=A4*A8*(CON5-CON4)*(A10*(11.D0-2.D0*ALAMDA*RA)*ALAMDA-2.D0*
     1(9.D0-2.D0*ALAMDA*RA))
C       XY-XZ  INTEGRAL
      EKS(8)=A8*A1*CON3*CON2*(-4.5D0+ALAMDA*(11.D0*CON4+RA)-2.D0*A13*CON
     14*RA)
C         XY-(X**2-Y**2) INTEGRAL
      EKS(9)=A9*A3*CON1*CON2*((CON4-CON5)*(11.D0-2.D0*ALAMDA*RA))
C       YZ-(3Z**2-R**2) INTEGRAL
      EKS(10)=A8*A2*CON2*CON3*(-A11+A10*(2.D0*A13*RA-11.D0
     1*ALAMDA))
C       XZ-(3Z**2-R**2) INTEGRAL
      EKS(11)=A8*A2*CON1*CON3*(-A11+A10*(2.D0*A13*RA-11.D0*ALAMDA))
C       XY-(3Z**2-R**2) INTEGRAL
      EKS(12)=A8*A2*CON1*CON2*(18.D0-11.D0*ALAMDA*A10-4.D0*ALAMDA*RA
     1+2.D0*A13*RA*A10)
C       XY-YZ INTEGRAL
      EKS(13)=A8*A1*CON1*CON3*(-0.5D0*A11+11.D0*CON5*ALAMDA-2.D0*
     1A13*CON5*RA)
C       YZ-(X**2-Y**2) INTEGRAL
      EKS(14)=A8*A3*CON2*CON3*(A11+(CON4-CON5)*(9.D0*ALAMDA-
     12.D0*A13*RA)+2.D0*ALAMDA*(CON4-CON5))
C       XZ-(X**2-Y**2) INTEGRAL
      EKS(15)=A8*A3*CON1*CON3*(-A11+(CON4-CON5)*(9.D0*ALAMDA-
     12.D0*A13*RA)+2.D0*ALAMDA*(CON4-CON5))
   50 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE R2
C       THIS SUBROUTINE CALCULATES THE R**2 INTEGRALS
      IMPLICIT REAL*8(A-F,H,O-Z)
      DIMENSION S(20),EKS(20),RSQU(15)
      COMMON CON1,CON2,CON3,CON4,CON5,CON6,S,RSQU,EKS,RAB,ALPHA1,
     1ALPHA2,RS,AI,AJ,AK,AX,AY,AZ,BX,BY,BZ,CX,CY,CZ,ALAMDA,ADELTA,
     2AZETA,U,PI,N
      A1=1.19366207
      A2=1.03374168/3.D0
      A3=0.59683104
      A4=0.51687084/3.D0
      A5=0.29841552
      A6=0.89524655/9.D0
      W=1.D0/(ALPHA1+ALPHA2)
      A7=ADELTA*AZETA*W**3
      A8=ALPHA2*W*A7
      A9=3.5D0+ALPHA2**2*W*RAB**2
      B1=CON4-CON5
      B2=CON4+CON5
      B3=A9*ALPHA1-ALPHA2
      B4=2.D0*ALAMDA
      B5=CON4+CON5-2.D0*CON6
      B6=4.D0*B2-8.D0*CON6
      B7=ALPHA2**2*W
      B8=2.D0*ALAMDA**2
C       (3Z**2-R**2)-(3Z**2-R**2)    INTEGRAL
      RSQU(1)=0.25D0*A8*A6*((12.D0/ALAMDA-8.D0*(CON4+CON5+4.D0*CON6)
     1 +ALAMDA*4.D0*B5**2)*B3+ALPHA1*B7*(12.D0/ALAMDA**2-4.D0*B5**2))
C     XY-XY   INTEGRAL
      RSQU(2)=0.5D0*A8*A1*(B3*(1.D0-B4*CON5)*(1.D0/ALAMDA-2.D0*CON4)
     1+B7*(1.D0/ALAMDA**2-4.D0*CON4*CON5))
C       XZ-XZ  INTEGRAL
      RSQU(3)=0.5D0*A8*A1*(B3*(1.D0-B4*CON6)*(1.D0/ALAMDA-2.D0*CON4)
     1+B7*(1.D0/ALAMDA**2-4.D0*CON4*CON6))
C       YZ-YZ   INTEGRAL
```

```
      RSQU(4)=0.5D0*A8*A1*(B3*(1.D0-B4*CON6)*(1.D0/ALAMDA-2.D0*CON5)
     1+B7*(1.D0/ALAMDA**2-4.D0*CON5*CON6))
C       (X**2-Y**2)-(X**2-Y**2)  INTEGRAL
      RSQU(5)=A7*A5*((1.D0-B4*B2+0.5D0*B8*B1**2)*A9
     1+2.D0*B7*(B2-ALAMDA*B1**2))
C      YZ-XZ  INTEGRAL
      RSQU(6)=0.5D0*A8*A1*(CON1*CON2*(-1.D0+B4*CON6)*B3
     1-2.D0*B7*ALPHA1*CON1*CON2*CON6)
C       (X**2-Y**2)-(3Z**2-R**2)  INTEGRAL
      RSQU(7)=A8*A4*B1*(B3*(2.D0-ALAMDA*B5)+ALPHA1*B7*B5)
C       XY-XZ   INTEGRAL
      RSQU(8)=0.5D0*A8*A1*(CON2*CON3*(B4*CON4-1.D0)*B3
     1-2.D0*ALPHA1*B7*CON2*CON3*CON4)
C        XY-(X**2-Y**2)  INTEGRAL
      RSQU(9)=ALPHA1*ALPHA2*A3*A8*W*CON1*CON2*B1*(ALPHA1*A9
     1-2.D0*ALPHA2)
C       YZ-(3Z**2-R**2)  INTEGRAL
      RSQU(10)=A8*A2*CON2*CON3*((-1.D0-B5*ALAMDA)*B3+ALPHA1*B7*B5)
C       XZ-(3Z**2-R**2)  INTEGRAL
      RSQU(11)=A8*A2*CON1*CON3*((-1.D0-B5*ALAMDA)*B3+ALPHA1*B7*B5)
C       XY-(3Z**2-R**2)  INTEGRAL
      RSQU(12)=A8*A2*CON1*CON2*((2.D0-ALAMDA*B5)*B3+ALPHA1*B7*B5)
C       XY-YZ  INTEGRAL
      RSQU(13)=0.5D0*A8*A1*(CON1*CON3*(-1.D0+B4*CON5)*B3
     1-2.D0*ALPHA1*B7*CON1*CON3*CON5)
C       YZ-(X**2-Y**2)  INTEGRAL
      RSQU(14)=A8*A3*((1.D0+B1*ALAMDA)*B3-ALPHA1*B7*B1)*CON2*CON3
C       XZ-(X**2-Y**2)  INTEGRAL
      RSQU(15)=A8*A3*((-1.D0+B1*ALAMDA)*B3-ALPHA1*B7*B1)*CON1*CON3
      RETURN
      END
```

```
0.02706    0.14598    0.36418    0.45438    0.33310
```

```
DZ2DZ2DXYDXYDXZDXZDYZDYZDX2DX2DYZDZXDX2DZ2DXYDZXDXYDX2DYZDZ2DZXDZ2DXYDZ2DXYDYZ
DYZDX2DZXDX2
      1
 3.322
48.9403    0.27060000D-01
13.7169    0.14592000D 00
4.63951    0.36418000D 00
1.57433    0.46438000D 00
.486409    0.33310000D 00
      1      1
```

```
C       THIS PROGRAM COMPUTES THE TIGHT-BINDING MATRIX
C       ELEMENTS, EIGENVALUES, EIGENVECTORS, DENSITY OF
C       STATES, AND FERMI ENERGY FOR A FACE-CENTERED
C       CUBIC LATTICE
        REAL * 8  H,OV,XL,X1,CCV,C1V,C2V,C3V,SSV,S1V,S2V,
     1  S3V,V,C1,C2,C3,XK,YK,ZK,RMATX,T(750)
        REAL *8 P,CON,Q,PR,PS,HCC
        DIMENSION HCC(4,46)
        DIMENSION V(38,38,2),CON(74)
        DIMENSION IX(74),IY(74),IZ(74),ID(74)
        DIMENSION  H(38,38),OV(38,38),XL(38),X1(38,38)
        DIMENSION CCV(6),C3V(6),C2V(6),C1V(6),SSV(6),
     1    S3V(6),S2V(6),S1V(6)
        COMMON/LCS/DD(325,5,2),PD(2,40,25,9),PP(45,40,2),
     1    SD(2,40,25,4),
     *  SP(2,40,4,9),SS(10,40,2),SW(8,1500),EN(1500)
        COMMON  HCC,V,CON,CCV,C1V,C2V,C3V,SSV,S1V,S2V,S3V,
     1     Q,J,IDD,ISS,IPP,IPD,ISD,ISP
        EQUIVALENCE  (V(1,1,1),H(1,1)),(V(1,1,2),OV(1,1))
C        Q IS THE EXCHANGE PARAMETER
        Q=0.9718
        Q=2.0/3.0
C      MM15 IS 1 FOR PARA., 2 FOR UP, AND 3 FOR DOWN EXCH
        MM15=1
        MM15=2
        MM15=3
C        KMX IS THE KX COORDINATE AT SYMMETRY POINT X
        KMX=8
        RHO=5.0
        RHO=4.72
        RHO=5.28
        GO TO (23456,34567,45678),MM15
23456   WRITE(6,65432)  Q
65432   FORMAT(1X,'PARAMAGNETIC  NICKEL',5X,'Q=',E16.8)
        GO TO 56789
34567   WRITE(6,76543) Q
76543   FORMAT(1X,'UP SPIN EXCHANGE ',5X,'Q=',E16.8)
        GO TO 56789
45678   WRITE(6,87654) Q
87654   FORMAT(1X,'DOWN SPIN EXCHANGE ',5X,'Q=',E16.8)
56789   CONTINUE
C        PARAMETERS BELOW INDICATE THE NO. OF NEIGHBORS
C       FOR EACH TYPE OF INTEGRAL INDICATED
        IDD=5
        ISS=40
        IPP=40
        ISD=40
        ISP=40
        IPD=30
C        SET UP FOR ENERGY BINS TO CALCULATE THE DENSITY OF
C       STATES, WITH LOWER LIMIT OF EMIN, AT DEN INTERVALS,
C       WITH TOTAL NO. OF BINS EQUAL TO NEN.  EIGENVALUES
C       OF INTEREST ARE NB1 TO NB2.  SW(I,1500) HAS DENSITY
```

```
C       OF STATES FOR EACH OF SIX BANDS FOR I=1 TO 6, TOTAL
C       DENSITY OF STITES IN I=7, AND NO. OF ELECTRONS I=8
        EMIN=-1.25
        DEN=0.00055
        NEN=1500
        SUM=((FLOAT(KMX))**3)/12.
        NB1=24
        NB2=29
        XQ=EMIN-0.001
        DO 2010 I=1,NEN
        EN(I)=XQ
  2010  XQ=XQ+DEN
        DO 2011 I=1,8
        DO 2011 J=1,NEN
  2011  SW(I,J)=0.0
        A=1.0D-10
C        READ DIRECT LATTICE VECTORS
        READ(5,4080) (IX(J),J=1,74)
        READ(5,4080) (IY(J),J=1,74)
        READ(5,4080) (IZ(J),J=1,74)
  4080  FORMAT(20I2/20I2/20I2/14I2)
  9980  FORMAT(15I2)
        DO 4021 I15=1,4
        DO 4021 I16=1,46
  4021  HCC(I15,I16)=0.0
C        READ CENTRAL CELL (R=0) INTEGRALS
        DO 4020 I11=1,4
        NEND=46
        IF(I11.GE.3) NEND=31
        DO 4001 I10=1,NEND
  4001  READ(5,4000) HCC(I11,I10)
  4020  CONTINUE
  4000  FORMAT(E15.7)
        PQR=10.D-12
C        READ R=1, ETC  INTEGRALS IN READBD
        CALL READBD(MM15)
C        SET UP CONSTANTS CON WHICH ARE
C          (OCCUPATION OF SHELL) / 6.
        DO 101 J=1,74
        NPR=0
        NO=0
        IF(IX(J).EQ.0)NO=NO+1
        IF(IY(J).EQ.0)NO=NO+1
        IF(IZ(J).EQ.0)NO=NO+1
        IF(IX(J).EQ.IY(J))NPR=NPR+1
        IF(IX(J).EQ.IZ(J).OR.IY(J).EQ.IZ(J))NPR=NPR+1
        PR=4.D0*NPR-2.D0
        IF(NPR.EQ.0) PR=1.D0
        CON(J)=8.D0/(2.D0**NO*PR)
   101  CONTINUE
        NM=0
        NA=0
C        SET UP DO-LOOPS OVER K-SPACE, BOUNDED TO THE
```

```
C      IRREDUCIBLE 1/48 TH OF THE BRILLOUIN ZONE
C      FOR 89 POINTS, IE, X IS (8,0,0)
       DO 120 I1=1,9
       DO 120 I2=1,I1
       DO I3=1,I2
       KX=I1-1
       KY=I2-1
       KZ=I3-1
       LMN=KX+KY+KZ
       IF(LMN.GT.12) GO TO 120
       NM=NM+1
       XK=KX
       YK=KY
       ZK=KZ
       WRITE(6,222)XK,YK,ZK,NM
  222  FORMAT(30X,3HK=(,3F6.2,1H),5X,'NM=',I5)
       WRITE(6,221)
       XK=3.141592653589793*XK/4.0
       YK=3.141592653589793*YK/4.0
       ZK=3.141592653589793*ZK/4.0
       DO150J=1,2
       DO 150 K=1,38
       DO 150 L=1,38
  150  V(K,L,J)=0.0
C       START BY PLACING CENTRAL CELL INTEGRALS IN V(     )
       DO 4002 I11=1,3
       N=1
       P5=1.D0
       IF(I11.EQ.2) P5=Q
 4002  CALL CENT(N,P5,I11)
       N=2
       P5=1.D0
       CALL CENT(N,P5,4)
C       PERFORM SUM OVER DIRECT LATTICE (R I, I=1,40)
       DO 200 J=1,40
C       FIRST CALCULATE ALL ANGULAR PARAMETERS NEEDED
       C1=IX(J)
       C2=IY(J)
       C3=IZ(J)
       C1=C1/2.D0
       C2=C2/2.D0
       C3=C3/2.D0
       C1XK=DCOS(C1*XK)
       C3XK=DCOS(C3*XK)
       C2XK=DCOS(C2*XK)
       C1YK=DCOS(C1*YK)
       C2YK=DCOS(C2*YK)
       C3YK=DCOS(C3*YK)
       C1ZK=DCOS(C1*ZK)
       C2ZK=DCOS(C2*ZK)
       C3ZK=DCOS(C3*ZK)
       S1XK=DSIN(C1*XK)
       S2XK=DSIN(C2*XK)
```

```
S3XK=DSIN(C3*XK)
S1YK=DSIN(C1*YK)
S2YK=DSIN(C2*YK)
S3YK=DSIN(C3*YK)
S1ZK=DSIN(C1*ZK)
S2ZK=DSIN(C2*ZK)
S3ZK=DSIN(C3*ZK)
CCV(1)=C1XK*C2YK*C3ZK
CCV(2)=C1XK*C3YK*C2ZK
CCV(3)=C3XK*C2YK*C1ZK
CCV(4)=C3XK*C1YK*C2ZK
CCV(5)=C2XK*C1YK*C3ZK
CCV(6)=C2XK*C3YK*C1ZK
C1V(1)=C1XK*S2YK*S3ZK
C1V(2)=C1XK*S3YK*S2ZK
C1V(3)=C3XK*S2YK*S1ZK
C1V(4)=C3XK*S1YK*S2ZK
C1V(5)=C2XK*S1YK*S3ZK
C1V(6)=C2XK*S3YK*S1ZK
C2V(1)=S1XK*C2YK*S3ZK
C2V(2)=S1XK*C3YK*S2ZK
C2V(3)=S3XK*C2YK*S1ZK
C2V(4)=S3XK*C1YK*S2ZK
C2V(5)=S2XK*C1YK*S3ZK
C2V(6)=S2XK*C3YK*S1ZK
C3V(1)=S1XK*S2YK*C3ZK
C3V(2)=S1XK*S3YK*C2ZK
C3V(3)=S3XK*S2YK*C1ZK
C3V(4)=S3XK*S1YK*C2ZK
C3V(5)=S2XK*S1YK*C3ZK
C3V(6)=S2XK*S3YK*C1ZK
SSV(1)=S1XK*S2YK*S3ZK
SSV(2)=S1XK*S3YK*S2ZK
SSV(3)=S3XK*S2YK*S1ZK
SSV(4)=S3XK*S1YK*S2ZK
SSV(5)=S2XK*S1YK*S3ZK
SSV(6)=S2XK*S3YK*S1ZK
S3V(1)=C1XK*C2YK*S3ZK
S3V(2)=C1XK*C3YK*S2ZK
S3V(3)=C3XK*C2YK*S1ZK
S3V(4)=C3XK*C1YK*S2ZK
S3V(5)=C2XK*C1YK*S3ZK
S3V(6)=C2XK*C3YK*S1ZK
S2V(1)=C1XK*S2YK*C3ZK
S2V(2)=C1XK*S3YK*C2ZK
S2V(3)=C3XK*S2YK*C1ZK
S2V(4)=C3XK*S1YK*C2ZK
S2V(5)=C2XK*S1YK*C3ZK
S2V(6)=C2XK*S3YK*C1ZK
S1V(1)=S1XK*C2YK*C3ZK
S1V(2)=S1XK*C3YK*C2ZK
S1V(3)=S3XK*C2YK*C1ZK
S1V(4)=S3XK*C1YK*C2ZK
```

```
      S1V(5)=S2XK*C1YK*C3ZK
      S1V(6)=S2XK*C3YK*C1ZK
C       SUBROUTINE MATRIX PERFORMS SUM
  199 CALL MATRIX
 200  CONTINUE
      DO246 J=1,2
      DO 246 K=1,38
      DO 246 L=1,38
      B=V(K,L,J)
      IF(ABS(B).GT.POR) GO TO 246
      V(K,L,J)=0.0
  246 CONTINUE
      M=38
C       FROM HERE TO 7151, PERFORM DIAGONALIZATION OF
C      SECULAR EQUATION,  DET/H(K)-E S(K)/=0 YIELDING THE
C      ENERGY EIGENVALUES E.  PROCESS IS SERIES OF IBM
C      SCIENTIFIC SUBROUTINES DMFSD, DMTDS, AND DIGEN
C      DIGEN IS DOUBLE PRECISION VERSION OF EIGEN
      DO 7052 I=1,38
      DO 7052 J=1,I
      IJ=I*(I-1)/2+J
 7052 T(IJ)=OV(J,I)
      CALL DMFSD(T,38,A,IER)
      IF(IER.NE.0) GO TO 7200
      CALL DMTDS(H,38,38,T,-1,IER)
      IF(IER.NE.0) GO TO 7201
      CALL DMTDS(H,38,38,T,2,IER)
      IF(IER.NE.0) GO TO 7202
      GO TO 7053
 7200 WRITE(6,7301)
      STOP 5
 7201 WRITE(6,7302)
      STOP 5
 7202 WRITE(6,7303)
      STOP 5
 7301 FORMAT(1X,'IER NE 0 IN MFSD')
 7302 FORMAT(1X,' IER NE 0 IN MTDS, 1 ST RUN')
 7303 FORMAT(1X,' IER NE 0 IN MTDS, 2 ST RUN')
 7053 CONTINUE
      DO 7150 I=1,38
      DO 7150 J=1,I
      IJ=I*(I-1)/2+J
 7150 T(IJ)=H(J,I)
      CALL DIGEN(T,X1,38,0)
      DO 7151 I=1,38
      IJ=I*(I-1)/2+I
 7151 XL(I)=T(IJ)
      CALL DENS(NM,XL,KX,KY,KZ,KMX,WT,SUM,SW,EN,NEN,
     1   DEN,NB1,NB2)
      WRITE(6,235)(XL(J),J=1,10)
  235 FORMAT(1X,10F13.7)
      WRITE(6,235)(XL(J),J=11,20)
```

```
      WRITE(6,235) (XL(J),J=21,30)
      WRITE(6,235) (XL(J),J=31,38)
      WRITE(6,221)
  221 FORMAT(1H )
  120 CONTINUE
      CALL FERMI(SW,EN,RHO,NEN,NB1,NB2,DEN,EF)
      WRITE(6,11911) EF,RHO
11911 FORMAT(1X,'EF=',E16.8,'RHO=',E16.8)
      DO 11335 I1=1,1500
11335 WRITE(6,11336) EN(I1),(SW(I2,I1),I2=1,8)
11336 FORMAT(1X,9F10.6)
 9999 STOP
      END
      SUBROUTINE CENT(N,P,M)
C      THIS SUBROUTINE INSERTS CENTRAL CELL INTEGRALS
C     IN THE HAMILTONIAN H, AND OVERLAP S.
      REAL * 8  H,OV,XL,X1,CCV,C1V,C2V,C3V,SSV,S1V,S2V,
     1 S3V,V,C1,C2,C3,XK,YK,ZK,CON,HCC,Q,P,PT4,PT6,X,Y
      DIMENSION HCC(4,46),V(38,38,2)
      DIMENSION CON(74)
      DIMENSION CCV(6),C3V(6),C2V(6),C1V(6),SSV(6),
     1  S3V(6),S2V(6),S1V(6)
      COMMON/LCS/DD(325,5,2),PD(2,40,25,9),PP(45,40,2),
     1  SD(2,40,25,4),
     *  SP(2,40,4,9),SS(10,40,2),SW(8,1500),EN(1500)
      COMMON  HCC,V,CON,CCV,C1V,C2V,C3V,SSV,S1V,S2V,S3V,
     1     Q,J,IDD,ISS,IPP,IPD,ISD,ISP
      PT4=0.4D0
      PT6=0.6D0
      K=1
      DO 1 I=1,5
      DO 1 J=I,5
      L=31+K
C     X,Y ARE X-STAL FIELD SPLITTING IN D-D INTEGRALS
      X=HCC(M,K)*P+PT4*HCC(M,L)*P
      IA=I+5
      JA=J+5
      IB=I+10
      JB=J+10
      IC=I+15
      JC=J+15
      ID=I+20
      JD=J+20
      V(I,J,N)=X+V(I,J,N)
      V(IA,JA,N)=X+V(IA,JA,N)
      V(IB,JB,N)=X+V(IB,JB,N)
      Y=HCC(M,K)*P-PT6*HCC(M,L)*P
      V(IC,JC,N)=Y+V(IC,JC,N)
      V(ID,JD,N)=Y+V(ID,JD,N)
    1 K=K+1
      DO 2 I=26,29
      DO 2 J=I,29
      V(I,J,N)=V(I,J,N)+HCC(M,K)*P
```

```
    2 K=K+1
      DO 3 I=1,3
      DO 3 J=I,3
      IA=27+3*I
      JA=27+3*J
      IB=IA+1
      JB=JA+1
      IC=IB+1
      JC=JB+1
      V(IA,JA,N)=V(IA,JA,N)+HCC(M,K)*P
      V(IB,JB,N)=V(IB,JB,N)+HCC(M,K)*P
      V(IC,JC,N)=V(IC,JC,N)+HCC(M,K)*P
    3 K=K+1
      DO 250 I=1,2
      DO 250 L=1,38
      DO 250 LS=L,38
  250 V(LS,L,I)=V(L,LS,I)
      RETURN
      END
      SUBROUTINE MATRIX
C     MATRIX PERFORMS SUM OVER DIRECT LATTICE VECTORS
      REAL * 8  H,OV,XL,XI,CCV,C1V,C2V,C3V,SSV,S1V,S2V,
     1 S3V,V,C1,C2,C3,XK,YK,ZK,RMATX,Q,P,CON,OC,PT25,
     2  PT75,PT5,HCC
      DIMENSION V(38,38,2),CON(74),HCC(4,46)
      DIMENSION CCV(6),C3V(6),C2V(6),C1V(6),SSV(6),
     1  S3V(6),S2V(6),S1V(6)
      COMMON  HCC,V,CON,CCV,C1V,C2V,C3V,SSV,S1V,S2V,S3V,
     1    Q,J,IDD,ISS,IPP,IPD,ISD,ISP
      COMMON/LCS/DD(325,5,2),PD(2,40,25,9),PP(45,40,2),
     1 SD(2,40,25,4),
     *  SP(2,40,4,9),SS(10,40,2),SW(8,1500),EN(1500)
C      THE BASIS SET OF THE MATRIX IS D1 TO D5 XY, D1
C     TO D5 YZ, D1 TO D5 XZ,D1 TO D5 (X**2-Y**2), D1 TO
C     D5 (3Z**2-R**2), 1S, 2S, 3S, 4S, 2PX,2PY, 2PZ,
C     3PX, 3PY, 3PZ, 4PX, 4PY, 4PZ.  D1 TO D5 IMPLIES
C     5 INDIVIDUAL D-TYPE ORBITALS USED.
      P=DSQRT(3.D0)
      PT25=0.25D0
      PT75=0.75D0
      PT5=0.5D0
      OC=CON(J)
C      PERFORM SUM FOR H AND S
      DO210I=1,2
      IF(J.GT.IDD) GO TO 9010
C      D-D BLOCK HAS INDIVIDUAL ORBITALS, INTEGRALS STORED
C     IN TRIANGULAR PART OF 25 X 25 BLOCK
      DO 1000 M=1,5
      DO 1000 N=1,5
      NM=M*(M-1)/2+N
      NM5=(M+5)*(M+4)/2+N
      NM10=(M+10)*(M+9)/2+N
```

```
      NM15=(M+15)*(M+14)/2+N
      NM20=(M+20)*(M+19)/2+N
      N5M5=(M+5)*(M+4)/2+(N+5)
      N10M10=(M+10)*(M+9)/2+(N+10)
      N15M15=(M+15)*(M+14)/2+(N+15)
      N20M20=(M+20)*(M+19)/2+(N+20)
      N5M10=(M+10)*(M+9)/2+(N+5)
      N5M15=(M+15)*(M+14)/2+(N+5)
      N5M20=(M+20)*(M+19)/2+(N+5)
      N10M15=(M+15)*(M+14)/2+(N+10)
      N10M20=(M+20)*(M+19)/2+(N+10)
      N15M20=(M+20)*(M+19)/2+(N+15)
      IF(M.LT.N) GO TO 15
C       XY-XY
      V(N,M,I)=V(N,M,I)+OC*(DD( NM,J,I)*(CCV(1)
     1+CCV(5))+DD(N5M5,J,I    )*(CCV(3)+CCV(6))
     2+DD(N10M10,J,I     )*(CCV(2)+CCV(4)))
C       YZ-YZ
      V(N+5,M+5,I)=V(N+5,M+5,I)+OC*(DD(N5M5,J,I     )
     1*(CCV(1)+CCV(2))+DD(NM,J,I )*(CCV(3)+
     2CCV(4))+DD(N10M10,J,I     )*(CCV(5)+CCV(6)))
C       XZ-XZ
      V(N+10,M+10,I)=V(N+10,M+10,I)+OC*(DD(N10M10,J,I)
     1*(CCV(1)+CCV(3))+DD(N5M5,J,I     )*(CCV(5)+
     2CCV(4))+DD(NM,J,I )*(CCV(6)+CCV(2)))
C       (X**2-Y**2)-(X**2-Y**2)
      V(N+15,M+15,I)=V(N+15,M+15,I)+OC*(DD(N15M15,J,I)
     1*(CCV(1)+CCV(5)+PT25*(CCV(3)+CCV(6)+CCV(4)
     2+CCV(2)))+(0.75D0*DD(N20M20,J,I)+0.5D0*
     3P*DD(N15M20,J,I))*(CCV(3)+CCV(2)+
     1CCV(4)+CCV(6))-P*DD(N15M20,J,I     )*(CCV(2)+CCV(4)))
C       (3Z**2-R**2)-(3Z**2-R**2)
      V(N+20,M+20,I)=V(N+20,M+20,I)+OC*DD(N20M20,J,I)
     1*(CCV(1)+CCV(5)+PT25*CCV(3)+PT25*CCV(6)+PT25
     2*CCV(4)+PT25*CCV(2))+CON(J)*DD(N15M15,J,I)
     3*PT75*(CCV(3)+CCV(6)+CCV(2)+CCV(4))+CON(J)
     4*P*PT5*DD(N15M20,J,I     )*(-CCV(3)-CCV(6)
     5+CCV(4)+CCV(2))
C       (X**2-Y**2)-(3Z**2-R**2)
      V(N+15,M+20,I)=V(N+15,M+20,I)+OC*(DD(N15M20,J,I)
     1*(CCV(1)-CCV(5)+PT5*CCV(2)-PT5*CCV(4)
     2+PT5*CCV(3)-PT5*CCV(6))+P*PT25*(DD(N20M20,J,I)
     3-DD(N15M15,J,I     ))*(CCV(2)-CCV(4)+CCV(6)
     4-CCV(3)))
      V(M+15,N+20,I)=V(N+15,M+20,I)
   15 CONTINUE
C       XY-YZ
      V(N,M+5,I)=V(N,M+5,I)-OC*(DD(NM5,J,I    )*(C2V(1)
     1+C2V(3))+DD(NM10,J,I    )*(C2V(5)+C2V(4))
     2+DD(N5M10,J,I     )*(C2V(2)+C2V(6)))
C       XY-XZ
      V(N,M+10,I)=V(N,M+10,I)-OC*(DD(NM10,J,I)
     1*(C1V(1)+C1V(2))+DD(N5M10,J,I     )*(C1V(4)
```

```
      2+C1V(3))+DD(NM5,J,I   )*(C1V(5)+C1V(6)))
C       XY-(X**2-Y**2)
       V(N,M+15,I)=V(N,M+15,I)+OC*(DD(NM15,J,I)
      1*(-C3V(1)+C3V(5))+PT5*(P*DD(N5M20,J,I)
      2+DD(N5M15,J,I    ))*(-C3V(3)+C3V(6))
      3+PT5*(P*DD(N10M20,J,I    )-DD(N10M15,J,I))
      4*(C3V(2)-C3V(4)))
C       XY-(3Z**2-R**2)
       V(N,M+20,I)=V(N,M+20,I)+OC*(DD(NM20,J,I)
      1*(-C3V(1)-C3V(5))+PT5*(DD(N5M20,J,I)
      2-P*DD(N5M15,J,I))*(C3V(3)+C3V(6))
      3+PT5*(DD(N10M20,J,I    )+P*DD(N10M15,J,I))
      4*(C3V(4)+C3V(2)))
C       YZ-XZ
       V(N+5,M+10,I)=V(N+5,M+10,I)+OC*(DD(N5M10,J,I)
      1*(-C3V(1)-C3V(5))-DD(NM5,J,I   )*(C3V(2)
      2+C3V(4))-DD(NM10,J,I   )*(C3V(3)+C3V(6)))
C       YZ-(X**2-Y**2)
       V(N+5,M+15,I)=V(N+5,M+15,I)+OC*(DD(N5M15,J,I)
      1*(-C1V(1)-PT5*C1V(2))+DD(N10M15,J,I)
      2*(C1V(5)+PT5*C1V(6))-PT5*P*DD(NM20,J,I)
      3*(C1V(3)+C1V(4))-PT5*DD(NM15,J,I)
      4*(C1V(3)-C1V(4))+P*PT5*(DD(N10M20,J,I)
      5*C1V(6)+DD(N5M20,J,I    )*C1V(2)))
C       YZ-(3Z**2-R**2)
       V(N+5,M+20,I)=V(N+5,M+20,I)+OC*(DD(N5M20,J,I)*(-C1V
      I(1))-DD(N10M20,J,I)*C1V(5)+PT5*(DD(NM20,J,I)-P*
      2DD(NM15,J,I))*C1V(3)+PT5*(DD(N10M20,J,I)-P*DD(
      3N10M15,J,I))*C1V(6)+PT5*(DD(N5M20,J,I)+P*DD(N5M15,
      4J,I))*C1V(2)+PT5*(DD(NM20,J,I)+P*DD(NM15,J,I))
      5 *C1V(4))
C       XZ-(X**2-Y**2)
       V(N+10,M+15,I)=V(N+10,M+15,I)+OC*(DD(N10M15,J,I)
      1*(-C2V(1)-PT5*C2V(3))+DD(N5M15,J,I)
      2*(C2V(5)+PT5*C2V(4))-P*PT5*DD(N10M20,J,I)
      3*C2V(3)-P*PT5*C2V(4)*DD(N5M20,J,I)
      4+P*PT5*DD(NM20,J,I   )*(C2V(6)+C2V(2))
      5+PT5*DD(NM15,J,I   )*(C2V(6)-C2V(2)))
C       XZ-(3Z**2-R**2)
       V(N+10,M+20,I)=V(N+10,M+20,I)+OC*(DD(N10M20,J,I)
      1*(-C2V(1)+PT5*C2V(3))-DD(N5M20,J,I)
      2*(C2V(5)-PT5*C2V(4))+PT5*DD(NM20,J,I)
      3*(C2V(2)+C2V(6))+P*PT5*DD(N5M15,J,I)
      4*C2V(4)-P*PT5*DD(N10M15,J,I    )*C2V(3)
      5+P*PT5*DD(NM15,J,I   )*(C2V(2)-C2V(6)))
 1000 CONTINUE
 9010 CONTINUE
      IF(J.GT.IPD) GO TO 77877
C       PD BLOCK HAS H AND S, 40 NEIGHBORS, AND 25 X 9
C      MATRIX BLOCK, 9 COMES FROM 2P, 3P, 4P, EACH WITH
C      X,Y, Z SYMMETRY.  KK=1 2P, KK=2 3P, AND KK=3 4P
      DO 4050 KK=1,7,3
      DO 4050 L=1,5
```

```
      K=KK+29
C       XY-X
      V(L,K,I)=V(L,K,I)+CON(J)*(PD(I,J,L,KK)
     1*S2V(1)+PD(I,J,L,KK+1)*S2V(5)
     2+PD(I,J,L+5,KK+2)*S2V(3)+PD(I,J,L+5,KK+1)
     3*S2V(6)+PD(I,J,L+10,KK)*S2V(2)
     4+PD(I,J,L+10,KK+2)*S2V(4))
C       YZ-X
      V(L+5,K,I)=V(L+5,K,I)-CON(J)*(PD(I,J,L+5,KK)
     1*(SSV(1)+SSV(2))+PD(I,J,L,KK+2)
     2*(SSV(3)+SSV(4))+PD(I,J,L+10,KK+1)*(SSV(5)+SSV(6)))
C       XZ-X
      V(L+10,K,I)=V(L+10,K,I)+CON(J)*(PD(I,J,L+10,KK)
     1*S3V(1)+PD(I,J,L+5,KK+1)*S3V(5)
     2+PD(I,J,L+10,KK+2)*S3V(3)+PD(I,J,L,KK+1)
     3*S3V(6)+PD(I,J,L,KK)*S3V(2)
     4+PD(I,J,L+5,KK+2)*S3V(4))
C       (X**2-Y**2)-X
      V(L+15,K,I)=V(L+15,K,I)+CON(J)*(PD(I,J,L+15,KK)
     1*S1V(1)-PD(I,J,L+15,KK+1)*S1V(5)+PT5
     2*(P*PD(I,J,L+20,KK+2)+PD(I,J,L+15,KK+2))*S1V(3)
     3-PT5*(P*PD(I,J,L+20,KK+1)+PD(I,J,L+15,KK+1))*S1V(6)
     4+PT5*(-P*PD(I,J,L+20,KK)+PD(I,J,L+15,KK))*S1V(2)
     5+PT5*(P*PD(I,J,L+20,KK+2)-PD(I,J,L+15,KK+2))*S1V(4))
C       (3Z**2-R**2)-X
      V(L+20,K,I)=V(L+20,K,I)+CON(J)*(PD(I,J,L+20,KK)
     1*S1V(1)+PD(I,J,L+20,KK+1)*S1V(5)-PT5
     2*(PD(I,J,L+20,KK+2)-P*PD(I,J,L+15,KK+2))
     3*S1V(3)-PT5*(PD(I,J,L+20,KK+1)-P*PD(I,J,L+15,KK+1))
     4*S1V(6)-PT5*(PD(I,J,L+20,KK)+P*PD(I,J,L+15,KK))
     5*S1V(2)-PT5*(PD(I,J,L+20,KK+2)+P*PD(I,J,L+15,
     6  KK+2))*S1V(4))
C       XY-Y
      V(L,K+1,I)=V(L,K+1,I)+CON(J)*(PD(I,J,L,KK+1)*S1V(1)
     1+PD(I,J,L,KK)*S1V(5)+PD(I,J,L+5,KK+1)*S1V(3)
     2+PD(I,J,L+5,KK+2)*S1V(6)+PD(I,J,L+10,KK+2)*S1V(2)
     3+PD(I,J,L+10,KK)*S1V(4))
C       YZ-Y
      V(L+5,K+1,I)=V(L+5,K+1,I)+CON(J)*(PD(I,J,L+5,KK+1)
     1*S3V(1)+PD(I,J,L+10,KK)*S3V(5)+PD(I,J,L,KK+1)
     2*S3V(3)+PD(I,J,L+10,KK+2)*S3V(6)+PD(I,J,L+5,KK+2)
     3*S3V(2)+PD(I,J,L,KK)*S3V(4))
C       XZ-Y
      V(L+10,K+1,I)=V(L+10,K+1,I)-CON(J)*(PD(I,J,L+10,
     1KK+1)*(SSV(1)+SSV(3))+PD(I,J,L,KK+2)*(SSV(2)+SSV(6))
     2+PD(I,J,L+5,KK)*(SSV(4)+SSV(5)))
C       (X**2-Y**2)-Y
      V(L+15,K+1,I)=V(L+15,K+1,I)+CON(J)*(PD(I,J,L+15,KK
     1+1)*S2V(1)-PD(I,J,L+15,KK)*S2V(5)+PT5*(P*
     2PD(I,J,L+20,KK+1)+PD(I,J,L+15,KK+1))*S2V(3)
     3-PT5*(P*PD(I,J,L+20,KK+2)+PD(I,J,L+15,KK+2))
     4*S2V(6)+PT5*(-P*PD(I,J,L+20,KK+2)+PD(I,J,L+15,
     *  KK+2))*S2V(2)+PT5*(P
```

```
      5*PD(I,J,L+20,KK)-PD(I,J,L+15,KK))*S2V(4))
C       (3Z**2-R**2)-Y
       V(L+20,K+1,I)=V(L+20,K+1,I)+CON(J)*(PD(I,J,L+20,KK
      1+1)*S2V(1)+PD(I,J,L+20,KK)*S2V(5)-PT5*
      2(PD(I,J,L+20,KK+1)-P*PD(I,J,L+15,KK+1))*S2V(3)
      3-PT5*(PD(I,J,L+20,KK+2)-P*PD(I,J,L+15,KK+2))
      4*S2V(6)-PT5*(PD(I,J,L+20,KK+2)+P*PD(I,J,L+15,
      *  KK+2))*S2V(2)-PT5*
      5(PD(I,J,L+20,KK)+P*PD(I,J,L+15,KK))*S2V(4))
C       XY-Z
       V(L,K+2,I)=V(L,K+2,I)-CON(J)*(PD(I,J,L,KK+2)
      1*(SSV(1)+SSV(5))+PD(I,J,L+5,KK)*(SSV(3)
      2+SSV(6))+PD(I,J,L+10,KK+1)*(SSV(2)+SSV(4)))
C       YZ-Z
       V(L+5,K+2,I)=V(L+5,K+2,I)+CON(J)*(PD(I,J,L+5,KK+2)
      1*S2V(1)+PD(I,J,L+10,KK+2)*S2V(5)
      2+PD(I,J,L,KK)*S2V(3)+PD(I,J,L+10,KK)*S2V(6)
      3+PD(I,J,L+5,KK+1)*S2V(2)+PD(I,J,L,KK+1)*S2V(4))
C       XZ-Z
       V(L+10,K+2,I)=V(L+10,K+2,I)+CON(J)*(PD(I,J,L+10,KK
      1+2)*S1V(1)+PD(I,J,L+5,KK+2)*S1V(5)+PD(I,J,L+10,KK)
      2*S1V(3)+PD(I,J,L,KK)*S1V(6)+PD(I,J,L,KK+1)*S1V(2)
      3+PD(I,J,L+5,KK+1)*S1V(4))
C       (X**2-Y**2)-Z
       V(L+15,K+2,I)=V(L+15,K+2,I)+CON(J)*(PD(I,J,L+15,KK
      1+2)*(S3V(1)-S3V(5))+PT5*(PD(I,J,L+20,KK)*P
      2+PD(I,J,L+15,KK))*(S3V(3)-S3V(6))+PT5*(-P*PD(I,J,L
      1 +20,KK+1)+PD(I,J,L+15,KK+1))*(S3V(2)-S3V(4)))
C       (3Z**2-R**2)-Z
       V(L+20,K+2,I)=V(L+20,K+2,I)+CON(J)*(PD(I,J,L+20,KK
      1+2)*(S3V(1)+S3V(5))+PT5*(P*PD(I,J,L+15,KK)
      2-PD(I,J,L+20,KK))*(S3V(3)+S3V(6))-PT5*(PD(I,J,
      4L+20,KK+1)+P*PD(I,J,L+15,KK+1))*(S3V(2)+S3V(4)))
 4050  CONTINUE
77877  CONTINUE
       IF(J.GT.ISD) GO TO 77977
C       SD HAS H AND S, 40 NEIGHBORS, AND 25 X 4 BLOCK,
C      THE 4 INDICATING 1S, 2S, 3S, 4S
       DO 3010 K=1,5
       DO 3010 L=1,4
C       XY-S
       V(K,L+25,I)=V(K,L+25,I)-CON(J)
      1*(SD(I,J,K,L)*(C3V(1)+C3V(5))
      2+SD(I,J,K+5,L)*(C3V(6)+C3V(3))
      3+SD(I,J,K+10,L)*(C3V(2)+C3V(4)))
C       YZ-S
       V(K+5,L+25,I)=V(K+5,L+25,I)-CON(J)
      1*(SD(I,J,K+5,L)*(C1V(1)+C1V(2))
      2+SD(I,J,K,L)*(C1V(3)+C1V(4))
      3+SD(I,J,K+10,L)*(C1V(5)+C1V(6)))
C       XZ-S
       V(K+10,L+25,I)=V(K+10,L+25,I)-CON(J)
      1*(SD(I,J,K+10,L)*(C2V(1)+C2V(3))
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     2+SD(I,J,K,L)*(C2V(2)+C2V(6))
     3+SD(I,J,K+5,L)*(C2V(5)+C2V(4)))
C      (X**2-Y**2)-S
      V(K+15,L+25,I)=V(K+15,L+25,I)+CON(J)*(SD(I,J,K+15,L)
     1*(CCV(1)-CCV(5))+(P*SD(I,J,K+20,L)+
     2SD(I,J,K+15,L))*PT5*(CCV(3)-CCV(6))-(P*SD(I,J,
     3K+20,L)-SD(I,J,K+15,L))*PT5*(CCV(2)-CCV(4)))
C      (3Z**2-R**2)-S
      V(K+20,L+25,I)=V(K+20,L+25,I)+CON(J)*(SD(I,J,K+20,
     1 L)*(CCV(1)+CCV(5)-PT5*(CCV(3)+CCV(6))-PT5*(CCV(2)
     3+CCV(4)))+SD(I,J,K+15,L)*P*PT5*(CCV(3)+CCV(6)
     4 -CCV(2)-CCV(4)))
 3010 CONTINUE
77977 CONTINUE
      IF(J.GT.ISS) GO TO 3001
C      SS IS 4 X 4 BLOCK STORED IN TRIANGULAR MODE
      DO 3000 K=26,29
      DO 3000 L=26,K
      KL=K-25
      LK=L-25
      IJ=KL*(KL-1)/2+LK
 3000 V(L,K,I)=V(L,K,I)+CON(J)*SS(IJ,J,I)
     1*(CCV(1)+CCV(2)+CCV(3)+CCV(4)+CCV(5)+CCV(6))
 3001 CONTINUE
      IF(J.GT.ISP) GO TO 3050
C      SP HAS H AND S, 40 NEIGHBORS, AND A 4 X 9 BLOCK
      DO 4000 K=1,7,3
      KK=K+29
      DO 4000 L=1,4
      LL=L+25
C      S-X
      V(LL,KK,I)=V(LL,KK,I)+CON(J)*(SP(I,J,L,K)
     1*(S1V(1)+S1V(2))+SP(I,J,L,K+2)
     2*(S1V(3)+S1V(4))+SP(I,J,L,K+1)*(S1V(5)+S1V(6)))
C      S-Y
      V(LL,KK+1,I)=V(LL,KK+1,I)+CON(J)
     1*(SP(I,J,L,K+1)*(S2V(1)+S2V(3))
     2+SP(I,J,L,K)*(S2V(5)+S2V(4))
     3+SP(I,J,L,K+2)*(S2V(2)+S2V(6)))
C      S-Z
      V(LL,KK+2,I)=V(LL,KK+2,I)+CON(J)
     1*(SP(I,J,L,K+2)*(S3V(1)+S3V(5))
     2+SP(I,J,L,K+1)*(S3V(4)+S3V(2))
     3+SP(I,J,L,K)*(S3V(6)+S3V(3)))
 4000 CONTINUE
 3050 CONTINUE
      IF(J.GT.IPP) GO TO 77677
C      PP IS 9 X 9 BLOCK STORED IN TRIANGULAR MODE
      DO 7000 K=1,7,3
      DO 7000 L=1,K,3
      LL=L+29
      KK=K+29
      LK=K*(K-1)/2+L
```

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      L2K2=(K+2)*(K+1)/2+(L+2)
      L1K1=((K+1)*K)/2+(L+1)
      LK2=(K+2)*(K+1)/2+L
      L1K2=(K+2)*(K+1)/2+(L+1)
      LK1=((K+1)*K)/2+L
C       X-X
      V(LL,KK,I)=V(LL,KK,I)+CON(J)*(PP(LK,J,I)*(CCV(1)
     1+CCV(2))+PP(L2K2,J,I)*(CCV(3)+CCV(4))
     2+PP(L1K1,J,I)*(CCV(5)+CCV(6)))
C       Y-Y
      V(LL+1,KK+1,I)=V(LL+1,KK+1,I)+CON(J)*(PP(L1K1,J,I)
     1*(CCV(1)+CCV(3))+PP(LK,J,I)*(CCV(5)+CCV(4))
     2+PP(L2K2,J,I)*(CCV(6)+CCV(2)))
C       Z-Z
      V(LL+2,KK+2,I)=V(LL+2,KK+2,I)+OC*(PP(L2K2,J,I)
     1*(CCV(1)+CCV(5))+PP(L1K1,J,I)*(CCV(2)+CCV(4))
     2+PP(LK,J,I)*(CCV(3)+CCV(6)))
C       K EQ L IMPLIES A DIAGONAL SUBBLOCK SUCH AS 2P-2P,
C      THEREFORE ONLY NEED X-Y AND NOT X-Y PLUS Y-X
      IF(K.EQ.L) GO TO 10
      L1K=K*(K-1)/2+L+1
      L2K=K*(K-1)/2+L+2
      L2K1=K*(K+1)/2+L+2
C       X-Y
      V(LL,KK+1,I)=V(LL,KK+1,I)-OC*(PP(LK1,J,I)*C3V(1)+
     1 PP(L1K,J,I)*C3V(5)+PP(L1K2,J,I)*C3V(6)+PP(L2K1,J,
     2 I)*C3V(3)+PP(LK2,J,I)*C3V(2)+PP(L2K,J,I)*C3V(4))
C       X-Z
      V(LL,KK+2,I)=V(LL,KK+2,I)-OC*(PP(LK2,J,I)*C2V(1)+
     1 PP(L2K,J,I)*C2V(3)+PP(L1K2,J,I)*C2V(5)+PP(L2K1,J,I)
     2 *C2V(4)+PP(LK1,J,I)*C2V(2)+PP(L1K,J,I)*C2V(6))
C       Y-Z
      V(LL+1,KK+2,I)=V(LL+1,KK+2,I)-OC*(PP(L1K2,J,I)*
     1 C1V(1)+PP(L2K1,J,I)*C1V(2)+PP(LK2,J,I)*C1V(5)+PP(
     2L2K,J,I)*C1V(6)+PP(LK1,J,I)*C1V(4)+PP(L1K,J,I)*
     3 C1V(3))
C       Y-X
      V(LL+1,KK,I)=V(LL+1,KK,I)-OC*(PP(LK1,J,I)*C3V(5)+
     1PP(L1K,J,I)*C3V(1)+PP(L1K2,J,I)*C3V(3)+PP(L2K1,J,I)
     2*C3V(6)+PP(LK2,J,I)*C3V(4)+PP(L2K,J,I)*C3V(2))
C       Z-X
      V(LL+2,KK,I)=V(LL+2,KK,I)-OC*(PP(LK2,J,I)*C2V(3)+PP
     1(L2K,J,I)*C2V(1)+PP(L1K2,J,I)*C2V(4)+PP(L2K1,J,I)
     2*C2V(5)+PP(LK1,J,I)*C2V(6)+PP(L1K,J,I)*C2V(2))
C       Z-Y
      V(LL+2,KK+1,I)=V(LL+2,KK+1   ,I)-OC*(PP(L1K2,J,I)*
     1*C1V(2)+PP(L2K1,J,I)*C1V(1)+PP(LK2,J,I)*C1V(6)+
     2PP(L2K,J,I)*C1V(5)+PP(LK1,J,I)*C1V(3)+PP(L1K,J,I)
     3 *C1V(4))
      GO TO 11
   10 CONTINUE
C       X-Y
      V(LL,KK+1,I)=V(LL,KK+1,I)-CON(J)*(PP(LK1,J,I)
```

```
     1*(C3V(1)+C3V(5))+PP(L1K2,J,I)*(C3V(3)+C3V(6))
     2+PP(LK2,J,I)*(C3V(2)+C3V(4)))
C      X-Z
      V(LL,KK+2,I)=V(LL,KK+2,I)-OC*(PP(LK2,J,I)
     1*(C2V(1)+C2V(3))+PP(L1K2,J,I)*(C2V(5)+C2V(4))
     2+PP(LK1,J,I)*(C2V(2)+C2V(6)))
C      Y-Z
      V(LL+1,KK+2,I)=V(LL+1,KK+2,I)-OC*(PP(L1K2,J,I)
     1*(C1V(1)+C1V(2))+PP(LK2,J,I)*(C1V(6)+C1V(5))
     2+PP(LK1,J,I)*(C1V(4)+C1V(3)))
   11 CONTINUE
 7000 CONTINUE
77677 CONTINUE
      DO 250 L=1,38
      DO 250 M=L,38
  250 V(M,L,I)=V(L,M,I)
 210  CONTINUE
      RETURN
      END
      SUBROUTINE DENS(   XL,KX,KY,KZ,KM,WT,SUM,SW,E,
     1   NEI,DE,NB1,NB2)
C      THIS SUBROUTINE CALCULATES THE WEIGHT OF EACH K
C     POINT AND THE DENSITY OF STATES OF EACH BAND
      REAL *8 XL
      DIMENSION SW(8,1500),E(1500),XL(38)
      KMA=3*KM/2
      IF(KX+KY+KZ-12 )17,23,23
 17   WT=1.
      IF(KX.EQ.KM)GOTO21
      IF(KZ.NE.0)GOTO19
      WT=WT*.5
      IF(KY.NE.0)GOTO18
      WT=WT*.25
      IF(KX.NE.0)GOTO28
      WT=WT*.16666667
      GOTO28
 18   IF(KX.NE.KY)GOTO28
      WT=WT*.5
      GOTO28
 19   IF(KY.NE.KZ)GOTO20
      WT=WT*.5
      IF(KX.NE.KY)GOTO28
      WT=WT*.33333333
      GOTO28
 20   IF(KX.NE.KY)GOTO28
      WT=WT*.5
      GOTO28
 21   WT=WT*.5
      IF(KZ.NE.0)GOTO22
      WT=WT*.5
      IF(KY.NE.0)GOTO28
      WT=WT*.25
      GOTO28
```

```
 22     IF(KY.NE.KZ)GOTO28
        WT=WT*.5
        GOTO28
 23     WT=.5
        IF(KX.EQ.KM)GOTO26
        IF(KZ.NE.0)GOTO24
        WT=WT*.5
        IF(KX.NE.KY)GOTO28
        WT=WT*.5
        GOTO28
 24     IF(KY.NE.KZ)GOTO25
        WT=WT*.5
        IF(KX.NE.KY)GOTO28
        WT=WT*.33333333
        GOTO28
 25     IF(KX.NE.KY)GOTO28
        WT=WT*.5
        GOTO28
 26     WT=WT*.5
        IF(KZ.NE.0)GOTO27
        WT=WT*.5
 27     IF(KY.NE.KZ)GOTO28
        WT=WT*.5
 28     CONTINUE
        WZ=WT/(SUM*DE)
        DO 36 KK=NB1,NB2
        K=KK-NB1+1
        DO 34 J=2,NEI
        M=J-1
        IF(XL(KK).GT.E(M).AND.XL(KK).LE.E(J))  GO TO 35
     34 CONTINUE
     35 SW(K,M)=SW(K,M)+WZ
     36 CONTINUE
        RETURN
        END
        SUBROUTINE FERMI(SW,E,DED,NEI,NB1,NB2,DE,EF)
C        THIS SUBROUTINE SUMS THE DENSITY OF STATES FOR
C       EACH BAND TO THE TOTAL DENSITY OF STATES AND
C       CALCULATES THE FERMI ENERGY BY COUNTING
C          ELECTRONS IN EACH ENERGY BIN
        DIMENSION SW(8,1500),E(1500)
        Q=0.0
        DO 39 J=1,NEI
        QA=0.0
        DO 38 I=1,6
     38 QA=QA+SW(I,J)
        SW(7,J)=QA
        Q=Q+QA*DE
     39 SW(8,J)=Q
        DO 41 J=2,NEI
        K=J-1
        IF(SW(8,K).LT.DED.AND.SW(8,J).GE.DED)GOTO40
        GOTO41
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 40     DRH=(SW(8,J)-SW(8,K))/DE
        EF=E(K)+(DED-SW(8,K))/DRH
        GOTO42
 41     CONTINUE
   42 RETURN
        END
        SUBROUTINE READBD(MM)
C        THIS SUBROUTINE READS ALL THE INTEGRALS NECESSARY
        REAL * 8  H,OV,XL,X1,CCV,C1V,C2V,C3V,SSV,S1V,S2V,
       1S3V,V,C1,C2,C3,XK,YK,ZK,P,CON,Q,PR,PS,HCC
        DIMENSION CCV(6),C3V(6),C2V(6),C1V(6),SSV(6),
       1 S3V(6),S2V(6),S1V(6)
        DIMENSION HCC(4,46),V(38,38,2),CON(74)
        COMMON  HCC,V,CON,CCV,C1V,C2V,C3V,SSV,S1V,S2V,S3V,
       1    Q,J,IDD,ISS,IPP,IPD,ISD,ISP
        COMMON/LCS/DD(325,5,2),PD(2,40,25,9),PP(45,40,2),
       1  SD(2,40,25,4),
       *  SP(2,40,4,9),SS(10,40,2),SW(8,1500),EN(1500)
        P=DSQRT(3.D0)
C        THE PARAMETER MM IS 1 FOR PARAMAGNETIC, 2 FOR
C       UP-SPIN, AND 3 FOR DOWN-SPIN EXCHANGE
        DO 4052 II=1,IDD
        DO 4052  JJ=1,325
        GO TO (11,12,13),MM
   11 READ(1) I,J,K    ,PO,EXCH,UP,DN,EK,OL,R2
        GO TO 14
   12 READ(1) I,J,K,PO,EXC,EXCH,DN,EK,OL,R2
        GO TO 14
   13 READ(1) I,J,K,PO,EXC,UP,EXCH,EK,OL,R2
   14 CONTINUE
        IF(ABS(PO).LT.10.D-15)  PO=0.0
        IF(ABS(EXCH).LT.10.D-15)  EXCH=0.0
        IF(ABS(EK).LT.10.D-15) EK=0.0
        IF(ABS(OL).LT.10.D-15)  OL=0.0
        JK=J*(J-1)/2+K
        DD(JK,I,1)=PO+EK+EXCH*Q
 4052 DD(JK,I,2)=OL
 4068 DO 4062 II=1,ISS
        DO 4062 JJ=1,10
        GO TO (21,22,23), MM
   21 READ(2) I,J,K,PO,EXCH,UP,DN,EK,OL,R2
        GO TO 24
   22 READ(2) I,J,K,PO,EXC,EXCH,DN,EK,OL,R2
        GO TO 24
   23 READ(2) I,J,K,PO,EXC,UP,EXCH,EK,OL,R2
   24 CONTINUE
        IF(ABS(PO).LT.10.D-15)  PO=0.0
        IF(ABS(EXCH).LT.10.D-15)  EXCH=0.0
        IF(ABS(EK).LT.10.D-15) EK=0.0
        IF(ABS(OL).LT.10.D-15)  OL=0.0
        J=J-25
        K=K-25
        JK=J*(J-1)/2+K
```

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      SS(JK,I,1)=PO+EK+EXCH*Q
 4062 SS(JK,I,2)=OL
 4066 DO 4054 II=1,IPP
      DO 4054 JJ=1,45
      GO TO (31,32,33), MM
   31 READ(3) I,J,K,PO,EXCH,UP,DN,EK,OL,R2
      GO TO 34
   32 READ(3) I,J,K,PO,EXC,EXCH,DN,EK,OL,R2
      GO TO 34
   33 READ(3) I,J,K,PO,EXC,UP,EXCH,EK,OL,R2
   34 CONTINUE
      IF(ABS(PO).LT.10.D-15)  PO=0.0
      IF(ABS(EXCH).LT.10.D-15)  EXCH=0.0
      IF(ABS(EK).LT.10.D-15) EK=0.0
      IF(ABS(OL).LT.10.D-15)  OL=0.0
      J=J-29
      K=K-29
      JK=J*(J-1)/2+K
      PP(JK,I,1)=PO+EK+EXCH*Q
 4054 PP(JK,I,2)=OL
 4067 DO 4056 II=1,IPD
      DO 4056 JJ=1,225
      GO TO (41,42,43), MM
   41 READ(4) I,J,K,PO,EXCH,UP,DN,EK,OL,R2
      GO TO 44
   42 READ(4) I,J,K,PO,EXC,EXCH,DN,EK,OL,R2
      GO TO 44
   43 READ(4) I,J,K,PO,EXC,UP,EXCH,EK,OL,R2
   44 CONTINUE
      IF(ABS(PO).LT.10.D-15)  PO=0.0
      IF(ABS(EXCH).LT.10.D-15)  EXCH=0.0
      IF(ABS(EK).LT.10.D-15) EK=0.0
      IF(ABS(OL).LT.10.D-15)  OL=0.0
      J=J-29
      PD(1,I,K,J)=PO+EK+EXCH*Q
 4056 PD(2,I,K,J)=OL
 4065 DO 4060 II=1,ISD
      DO 4060 JJ=1,100
      GO TO (81,82,83), MM
   81 READ(8) I,J,K,PO,EXCH,UP,DN,EK,OL,R2
      GO TO 84
   82 READ(8) I,J,K,PO,EXC,EXCH,DN,EK,OL,R2
      GO TO 84
   83 READ(8) I,J,K,PO,EXC,UP,EXCH,EK,OL,R2
   84 CONTINUE
      IF(ABS(PO).LT.10.D-15)  PO=0.0
      IF(ABS(EXCH).LT.10.D-15)  EXCH=0.0
      IF(ABS(EK).LT.10.D-15) EK=0.0
      IF(ABS(OL).LT.10.D-15)  OL=0.0
      J=J-25
      SD(1,I,K,J)=PO+EK+EXCH*Q
 4060 SD(2,I,K,J)=OL
      DO 4058 II=1,ISP
```

```
      DO 4058 JJ=1,36
      GO TO (91,92,93), MM
   91 READ(9) I,J,K,PO,EXCH,UP,DN,EK,OL,R2
      GO TO 94
   92 READ(9) I,J,K,PO,EXC,EXCH,DN,EK,OL,R2
      GO TO 94
   93 READ(9) I,J,K,PO,EXC,UP,EXCH,EK,OL,R2
   94 CONTINUE
      IF(ABS(PO).LT.10.D-15)  PO=0.0
      IF(ABS(EXCH).LT.10.D-15)  EXCH=0.0
      IF(ABS(EK).LT.10.D-15) EK=0.0
      IF(ABS(OL).LT.10.D-15)  OL=0.0
      J=J-29
      K=K-25
      SP(1,I,K,J)=PO+EK+EXCH*Q
 4058 SP(2,I,K,J)=OL
      RETURN
      END
C      IN THE CENTRAL CELL DATA BELOW, THE INTEGER ON
C     THE RIGHT IS 1 FOR COULOMB, 2 FOR EXCHANGE, 3 FOR
C     KINETIC ENERGY, AND 4 FOR OVERLAP.  THE SECOND
C     INTEGER HAS 1 FOR S-, 2 FOR P-, AND 3 FOR D-SYMMETRY
C     AND 4 FOR D-FIELD SPLITTING.  THE LAST TWO INTEGER
C     INDICATE SYMMETRY SUCH AS D1-D1, 1S-1S, ETC.  THE
C     EXCHANGE BELOW IS DOWN, AFTER // IS UP-SPIN EXCH.
```

```
1 0 1 2 3 2 3 0 1 3 4 3 2 4 5 5 4 3 5 4
0 5 1 6 5 2 6 4 7 5 5 6 7 5 3 6 7 6 7 0
1 7 5 8 4 6 6 2 7 8 7 6 7 8 9 3 8 9 7 5
6 9 8 7 9 7 4 7 9 8 0 8 1 7
1 0 1 2 1 2 2 0 1 3 2 3 2 3 1 2 4 3 3 4
0 3 1 2 4 2 3 4 1 5 4 4 2 5 3 4 3 5 3 0
1 4 5 2 4 5 6 2 5 3 4 6 5 4 1 3 4 2 6 5
6 3 5 5 3 6 4 7 4 5 0 6 1 7
0 2 2 0 0 2 1 4 4 0 0 2 4 1 0 1 0 4 0 2
6 2 6 0 1 6 1 4 0 0 3 0 1 2 6 2 0 1 2 8
8 1 4 0 6 3 0 8 0 1 3 2 2 0 0 8 2 1 1 6
4 0 1 4 2 3 8 0 1 310 010 2
-0.1875212E 03                           1    3    1    1
-0.6897548E 02                           1    3    1    2
-0.1584713E 02                           1    3    1    3
-0.2803761E 01                           1    3    1    4
-0.3809201E 00                           1    3    1    5
-0.6833014E 02                           1    3    2    2
-0.2902950E 02                           1    3    2    3
-0.6955805E 01                           1    3    2    4
-0.1070871E 01                           1    3    2    5
-0.2348073E 02                           1    3    3    3
-0.9000155E 01                           1    3    3    4
-0.1774529E 01                           1    3    3    5
-0.5990677E 01                           1    3    4    4
```

-0.1851814E 01	1	3	4	5
-0.1154503E 01	1	3	5	5
-0.1324310E 04	1	1	1	1
0.2727615E 03	1	1	1	2
-0.9898787E 02	1	1	1	3
0.2010376E 02	1	1	1	4
-0.2032222E 03	1	1	2	2
0.5673560E 02	1	1	2	3
-0.1127973E 02	1	1	2	4
-0.3361496E 02	1	1	3	3
0.6181469E 01	1	1	3	4
-0.2225997E 01	1	1	4	4
-0.1911322E 03	1	2	1	1
0.4503908E 02	1	2	1	2
-0.6725885E 01	1	2	1	3
-0.2761292E 02	1	2	2	2
0.3841836E 01	1	2	2	3
-0.1835243E 01	1	2	3	3
0.2401380E-03	1	4	1	1
-0.2504962E-06	1	4	1	2
-0.4202478E-06	1	4	1	3
-0.1451009E-06	1	4	1	4
-0.3974467E-08	1	4	1	5
-0.5781822E-05	1	4	2	2
-0.1348351E-04	1	4	2	3
-0.5956564E-05	1	4	2	4
-0.9416121E-06	1	4	2	5
-0.8012583E-04	1	4	3	3
-0.1187765E-03	1	4	3	4
-0.4457882E-04	1	4	3	5
-0.8119310E-03	1	4	4	4
-0.1126495E-02	1	4	4	5
-0.1084521E-01	1	4	5	5
-0.1345329E 02	2	3	1	1
-0.5796039E 01	2	3	1	2
-0.1399734E 01	2	3	1	3
-0.2526637E 00	2	3	1	4
-0.3456170E-01	2	3	1	5
-0.7621977E 01	2	3	2	2
-0.3935824E 01	2	3	2	3
-0.1051504E 01	2	3	2	4
-0.1698618E 00	2	3	2	5
-0.5057117E 01	2	3	3	3
-0.2661736E 01	2	3	3	4
-0.6131893E 00	2	3	3	5
-0.3054927E 01	2	3	4	4
-0.1304535E 01	2	3	4	5
-0.1383729E 01	2	3	5	5
-0.3130414E 02	2	1	1	1
0.3734298E 01	2	1	1	2
-0.1318769E 01	2	1	1	3
0.2669472E 00	2	1	1	4
-0.1168852E 02	2	1	2	2

0.1870434E 01	2	1	2	3
-0.3630292E 00	2	1	2	4
-0.4759300E 01	2	1	3	3
0.4989812E 00	2	1	3	4
-0.1229700E 01	2	1	4	4
-0.1262801E 02	2	2	1	1
0.1860759E 01	2	2	1	2
-0.2734389E 00	2	2	1	3
-0.4582089E 01	2	2	2	2
0.3963283E 00	2	2	2	3
-0.1243871E 01	2	2	3	3
-0.7452117E-05	2	4	1	1
-0.2362560E-07	2	4	1	2
0.8546952E-08	2	4	1	3
-0.5239320E-09	2	4	1	4
-0.8008053E-10	2	4	1	5
0.1084096E-06	2	4	2	2
-0.3500996E-07	2	4	2	3
-0.4408488E-07	2	4	2	4
-0.2602018E-08	2	4	2	5
-0.1866422E-07	2	4	3	3
-0.9622980E-08	2	4	3	4
-0.1321858E-08	2	4	3	5
-0.1153855E-04	2	4	4	4
-0.4458933E-03	2	4	4	5
-0.3597734E-01	2	4	5	5
0.3425818E 03	3	3	1	1
0.7716228E 02	3	3	1	2
0.7917941E 01	3	3	1	3
0.5283887E 00	3	3	1	4
0.2305401E-01	3	3	1	5
0.9601842E 02	3	3	2	2
0.2971268E 02	3	3	2	3
0.3461064E 01	3	3	2	4
0.1908482E 00	3	3	2	5
0.3247658E 02	3	3	3	3
0.1010240E 02	3	3	3	4
0.9501989E 00	3	3	3	5
0.1102031E 02	3	3	4	4
0.2936960E 01	3	3	4	5
0.3404865E 01	3	3	5	5
0.7571653E 03	3	1	1	1
-0.2770015E 03	3	1	1	2
0.1006100E 03	3	1	1	3
-0.2043947E 02	3	1	1	4
0.1427883E 03	3	1	2	2
-0.5842676E 02	3	1	2	3
0.1164197E 02	3	1	2	4
0.3040955E 02	3	1	3	3
-0.6690024E 01	3	1	3	4
0.1788424E 01	3	1	4	4
0.1401428E 03	3	2	1	1
-0.4648447E 02	3	2	1	2

0.6956669E 01	3	2	1	3
0.2695270E 02	3	2	2	2
-0.4243733E 01	3	2	2	3
0.1072335E 01	3	2	3	3
0.1000010E 01	4	3	1	1
0.5144238E 00	4	3	1	2
0.1334579E 00	4	3	1	3
0.2474452E-01	4	3	1	4
0.3419071E-02	4	3	1	5
0.1000000E 01	4	3	2	2
0.6121714E 00	4	3	2	3
0.1750540E 00	4	3	2	4
0.2901962E-01	4	3	2	5
0.9999999E 00	4	3	3	3
0.6138872E 00	4	3	3	4
0.1541644E 00	4	3	3	5
0.1000000E 01	4	3	4	4
0.5645410E 00	4	3	4	5
0.1000000E 01	4	3	5	5
0.9999844E 00	4	1	1	1
0.1201694E-04	4	1	1	2
-0.5822748E-05	4	1	1	3
-0.1331993E-04	4	1	1	4
0.9999973E 00	4	1	2	2
0.5364102E-05	4	1	2	3
-0.3661028E-05	4	1	2	4
0.9999881E 00	4	1	3	3
-0.7465015E-05	4	1	3	4
0.9999924E 00	4	1	4	4
0.9999818E 00	4	2	1	1
0.8009956E-06	4	2	1	2
0.1219881E-04	4	2	1	3
0.9999894E 00	4	2	2	2
-0.2330840E-02	4	2	2	3
0.9999995E 00	4	2	3	3

-0.1346846E 02	2	3	1	1
-0.5810759E 01	2	3	1	2
-0.1404386E 01	2	3	1	3
-0.2535896E 00	2	3	1	4
-0.3469362E-01	2	3	1	5
-0.7688931E 01	2	3	2	2
-0.3985085E 01	2	3	2	3
-0.1066150E 01	2	3	2	4
-0.1723109E 00	2	3	2	5
-0.5140411E 01	2	3	3	3
-0.2709108E 01	2	3	3	4
-0.6245061E 00	2	3	3	5
-0.3117829E 01	2	3	4	4
-0.1334229E 01	2	3	4	5
-0.1415957E 01	2	3	5	5

-0.3130498E 02	2	1	1	1
0.3732932E 01	2	1	1	2
-0.1318451E 01	2	1	1	3
0.2668849E 00	2	1	1	4
-0.1172486E 02	2	1	2	2
0.1856138E 01	2	1	2	3
-0.3601654E 00	2	1	2	4
-0.4830771E 01	2	1	3	3
0.5031542E 00	2	1	3	4
-0.1254350E 01	2	1	4	4
-0.1265581E 02	2	2	1	1
0.1846707E 01	2	2	1	2
-0.2713278E 00	2	2	1	3
-0.4652157E 01	2	2	2	2
0.4002088E 00	2	2	2	3
-0.1268995E 01	2	2	3	3
-0.7593575E-05	2	4	1	1
0.3165602E-08	2	4	1	2
0.1511992E-07	2	4	1	3
0.4039511E-09	2	4	1	4
0.2349412E-09	2	4	1	5
0.2532678E-06	2	4	2	2
0.7621259E-07	2	4	2	3
-0.4412666E-08	2	4	2	4
0.3462057E-08	2	4	2	5
0.9579151E-07	2	4	3	3
0.3833890E-07	2	4	3	4
0.7603609E-09	2	4	3	5
-0.1166220E-04	2	4	4	4
-0.4519355E-03	2	4	4	5
-0.3657290E-01	2	4	5	5

```
C       THIS PROGRAM OBTAINS THE SELF-CONSISTENT ENERGY
C       BANDS OF FERROMAGNETIC NICKEL
C       THIS PROGRAM SUMS SIJ OVER THE RECIPROCAL LATTICE
C       AND COMPUTES EIGENVALUES AND EIGENVECTORS FOR A
C       FACE-CENTERED CUBIC CRYSTAL.
        REAL*8 H,OV,XL,X1,T
        DIMENSION VK(51),RK(51),EK(741),OVR(741),T(741),
      1   H(38,38),XL(38),X1(38,38),DK(51),RSQ(741),NK(21),
      2   OV(38,38),XR(51),EVAL(10,38),POTE(741),EXCHE(741),
      3   CON(620)
        DIMENSION DUM1(51)
        DIMENSION EXC(741),HUP(741),HDN(741),DKUP(51),
      1 DKDN(51),XRUP(51),XRDN(51),RKUP(51),RKDN(51),
      2   VX0UP(51)
        COMMON/LCS/SIJ(51,741),VK0(620),VX0(620),VM(200),
      *   SW(8,3000),EN(3000),SWUP(8,3000),RHO0U(51),
      1 RHO0D(51),VM0(800),
      2   VW(200),IX(620),IY(620),IZ(620),IMAX,KKMAX
C
C
C       EF IS THE FERMI ENERGY AND FACT IS A PARAMETER TO
C       ACCELERATE CONVERGENCE
        EF=-1.021
        FACT=0.25
        RHO=5.0
        WRITE(6,22991) EF
22991   FORMAT(1X,'EF=',F8.4)
C       EMIN IS MINIMUM OF DENSITY OF STATES GRID (DESCRIBED
C       IN BAND PROGRAM ABOVE)
        EMIN=-2.08
        DEN=0.00055
        KMX=4
        NEN=3000
        SUM=((FLOAT(KMX))**3)/12.0
        NB1=24
        NB2=29
        A=1.0D-10
        READ(5,10000) NITER,IT,IOU,Q
C       NK ARE THE 20 POINTS OF THE 89 USED
        READ(5,8001) (NK(J),J=1,21)
 8001   FORMAT(21I2)
        ITER=1
        KNMAX=51
C       NITER IS NO. OF ITERATIONS IT AND IOU ARE DUMMY
C       VARIABLES, AND Q IS THE EXCHANGE PARAMETER, KNMAX
C       IS THE NO. OF RECIPROCAL LATTICE VECTORS TO CHANGE
        WRITE(6,10000) NITER,IT,KNMAX,Q,FACT
10000   FORMAT(3I5,2F9.5)
        KKMAX=619
        IMAX=193
        ACONST=6.644
        IX(1)=0
```

```
      IY(1)=0
      IZ(1)=0
      CON(1)=1.
      DO 380 IRLV=1,KNMAX
      RKUP(IRLV)=0.0
      RKDN(IRLV)=0.0
      XRUP(IRLV)=0.0
      XRDN(IRLV)=0.0
      RK(IRLV)=0.
      VK(IRLV)=0.
      XR(IRLV)=0.
  380 DK(IRLV)=0.
C     RHOOU AND RHOOD ARE THE FOURIER COEF OF THE COULOMB
C     POTENTIAL WHICH WILL BE USED TO GET CHARGE DENSITIES
C     FOR UP AND DOWN SPIN AT ZEROTH ITERATION
      DO 8002 I=1,51
 8002 READ(5,8003) RHOOU(I)
      DO 8004 I=1,51
 8004 READ(5,8003) RHOOD(I)
 8003 FORMAT(1X,E16.8)
C     READ IN CHANGES IN FOURIER COEF. FOR NEXT ITERATION
C     ( AT FIRST ITERATION, READ 27 BLANK CARDS)
      READ(5,236)(DK(IRLV),IRLV=1,KNMAX)
      READ(5,236) (XRUP(IRLV),IRLV=1,KNMAX)
      READ(5,236) (XRDN(IRLV),IRLV=1,KNMAX)
  236 FORMAT(6F13.7)
C     READ IN KNMAX FOURIER COEF.
      DO 3712 J=1,KNMAX
C    VKO IS COULOMB, VXOUP IS UP-SPIN AND VXO IS DOWN-SPIN
      READ(3) VKO(J),DUMMY,VXOUP(J),VXO(J),B,C,D,IOU
  393 FORMAT(1X,4E16.8,3F6.2,I5)
      K=B+.01
      L=C+.01
      M=D+.01
      ASQ=39.478418*(B*B+C*C+D*D)/ACONST**2
C     SUBTRACT OUT NUCLEAR TERMS
      IF(J.EQ.1)GO TO 3712
      ASQQ=25.132741*28.0/ASQ*4./ACONST**3
      RHOOU(J)=RHOOU(J)+ASQQ
      RHOOD(J)=RHOOD(J)+ASQQ
      VKO(J)=VKO(J)+ASQQ
C     CONVERT FROM V(K) TO RHO(K)
      ASQQ=-ASQ/25.132741
      RHOOU(J)=ASQQ*RHOOU(J)
      RHOOD(J)=ASQQ*RHOOD(J)
      VKO(J)=ASQQ*VKO(J)
C     SORT ASSURES K.GE.L.GE.M
      CALL SORT(K,L,M)
      IX(J)=K
      IY(J)=L
      IZ(J)=M
      II=K**2+L**2+M**2+1
      VMO(II)=VKO(J)
```

```
      IF(J.LE.KNMAX)VM(II)=VMO(II)-ASQ/25.132741*DK(J)
C     IOU IS THE OCCUPATION NO. OF R.L.V. IN UNIQUE SHELL
      CON(J)=IOU
      CON(J)=1./CON(J)
 3712 CONTINUE
      KSMAX=II
      PQR=10.0**(-13)
      VMO(1)=VKO(1)
      VM(1)=VKO(1)
C     READ FOURIER COEFFICIENTS FROM LAST ITERATION
  381 DO 382 IRLV=1,KNMAX
      VK(IRLV)=DK(IRLV)
      RKUP(IRLV)=RKUP(IRLV)+XRUP(IRLV)
      RKDN(IRLV)=RKDN(IRLV)+XRDN(IRLV)
      XR(IRLV)=0.
      DKUP(IRLV)=0.0
      DKDN(IRLV)=0.0
      XRUP(IRLV)=0.0
      XRDN(IRLV)=0.0
  382 DK(IRLV)=0.
      XQ=EMIN-0.001
      DO 2010I=1,NEN
      EN(I)=XQ
 2010 XQ=XQ+DEN
      DO 2011 I=1,8
      DO 2011 J=1,NEN
      SWUP(I,J)=0.0
 2011 SW(I,J)=0.0
      ATQ=0.
      SUMW=0.
      NM=0
C     THE FOLLOWING SET OF DO LOOPS ASSUMES THE
C     COORDINATES OF X TO BE 2*PI/(ICOR*A) * (ICOR,0,0)
C     DO LOOPS COVER 89 POINTS IN 1/48 TH  OF THE B.Z.
      BZU=0.0
      BZD=0.0
      BZ=0.0
      ICT=1
      ICOR=8
      NUT=ICOR/2+1
      MUT=3*ICOR/4+1
      LUT=ICOR+1
      DO 120 LU=1,LUT
      DO 120 MU=1,LU
      DO 120 NU=1,MU
      KX=LU-1
      KY=MU-1
      KZ=NU-1
      LMN=KX+KY+KZ
      IF(LMN.GT.3*ICOR/2)GO TO 120
      NM=NM+1
      NL=NM
      XK=KX
```

```
      YK=KY
      ZK=KZ
C     NEED MATRICES SUMMED OVER R FOR COULOMB POTENTIAL,
C     KINETIC ENERGY, OVERLAP,R SQUARED, AND EXCHANGE
C     POTENTIAL FOR UP-SPIN AND DOWN-SPIN
      DO 370 IBZ=1,741
      READ(1,9905) EK(IBZ),OVR(IBZ)
      READ(2,9905) POTE(IBZ),RSQ(IBZ)
C     READ EXCHANGE FOR UP AND DOWN
      READ(8,9905) EXC(IBZ),EXCHE(IBZ)
 9905 FORMAT(2A4)
      HUP(IBZ)=EK(IBZ)+POTE(IBZ)+Q*EXC(IBZ)
      HDN(IBZ)=EK(IBZ)+POTE(IBZ)+Q*EXCHE(IBZ)
  370 CONTINUE
      NL=NK(ICT)
C     READ SIJ BELOW ONLY FOR 20 K POINTS DONE
      IF(NM.NE.NL) GO TO 120
      ICT=ICT+1
C     WEIG FINDS WEIGHT OF EACH K POINT
      CALL WEIG(KX,KY,KZ,ICOR,WT)
      SUMW=SUMW+WT
      WRITE(6,222) XK,YK,ZK,NM,WT
  222 FORMAT(30X,'K=(',3F6.2,'H','  NM=',I5,' WT=',F8.5)
      XK=XK*3.14159265*2./ICOR
      YK=YK*3.14159265*2./ICOR
      ZK=ZK*3.14159265*2./ICOR
      DO 300 IRLV=1,KNMAX
      DO 300 I1=1,741
  300 READ(4,9) SIJ(IRLV,I1)
    9 FORMAT(A4)
      DO 120 IUD=1,2
      DO 733 IR=1,38
      DO 733 JR=1,IR
      IJ=JR+(IR*IR-IR)/2
  733 OV(IR,JR)=OVR(IJ)
      DO 327 I=1,38
      DO 327 J=1,38
  327 H(I,J)=0.
      DO 390 KN=1,KNMAX
      DO 390 I=1,38
      DO 390 J=1,I
      IJ=J+(I*I-I)/2
      GO TO (160,161),IUD
C     ONLY ADD IN CHANGE IN FOURIER COEFFICIENTS*SIJ
C     TO ZEROTH ORDER
  160 H(I,J)=H(I,J)+(VK(KN)+RKUP(KN)*Q)*SIJ(KN,IJ)
      GO TO 162
  161 H(I,J)=H(I,J)+(VK(KN)+RKDN(KN)*Q)*SIJ(KN,IJ)
  162 CONTINUE
  390 CONTINUE
      DO 391 I=1,38
      DO 391 J=1,I
      IJ=J+(I*I-I)/2
```

```
      GO TO (150,151),IUD
  150 H(I,J)=H(I,J)+HUP(IJ)
      GO TO 152
  151 H(I,J)=H(I,J)+HDN(IJ)
  152 OV(J,I)=OV(I,J)
  391 H(J,I)=H(I,J)
      J=38
C     TECHNIQUE BELOW TO DIAGONALIZE A MATRIX IS SAME
C     AS DESCRIBED IN BAND PROGRAM
  121 M=38
      A=10.**(-9)
      DO 7052 I=1,M
      DO 7052 J=1,I
      IJ=I*(I-1)/2+J
 7052 T(IJ)=OV(J,I)
      CALL DMFSD(T, M,A,IER)
      IF(IER.NE.0) GO TO 7200
      CALL DMTDS(H, M, M,T,-1,IER)
      IF(IER.NE.0) GO TO 7201
      CALL DMTDS(H, M, M,T,2,IER)
      IF(IER.NE.0) GO TO 7202
      GO TO 7053
 7200 WRITE(6,7301)
      STOP 5
 7201 WRITE(6,7302)
      STOP 5
 7202 WRITE(6,7303)
      STOP 5
 7301 FORMAT(1X,'IER NE 0 IN MFSD')
 7302 FORMAT(1X,' IER NE 0 IN MTDS, 1 ST RUN')
 7303 FORMAT(1X,' IER NE 0 IN MTDS, 2 ST RUN')
 7053 CONTINUE
      DO 7150 I=1,M
      DO 7150 J=1,I
      IJ=I*(I-1)/2+J
 7150 T(IJ)=H(J,I)
      CALL DIGEN(T,X1,M ,0)
      DO 7151 I=1,M
      IJ=I*(I-1)/2+I
 7151 XL(I)=T(IJ)
      DO 500 IR=1,M
      DO 500 JR=1,IR
      IJ=(IR*IR-IR)/2+JR
      OV(IR,JR)=OVR(IJ)
  500 OV(JR,IR)=OV(IR,JR)
      IF(NM.EQ.1) EMIN=XL(29)-0.05
      DO 502 L=1,M
      QN=0.
      DO 501 IR=1,M
      DO 501 JR=1,M
  501 QN=QN+X1(IR,L)*OV(IR,JR)*X1(JR,L)
      DO 502 IR=1,M
      IF(ITER.GT.10)GO TO 502
```

```
      IF(NM.NE.1)GO TO 502
      EVAL(ITER,IR)=XL(IR)
  502 X1(IR,L)=X1(IR,L)/SQRT(QN)
  123 WRITE(6,221)
      WRITE(6,235) (XL(J),J=1,38)
  235 FORMAT(1X,10F13.7)
  221 FORMAT(1H )
      WRITE(6,221)
      WRITE(6,221)
  122 MN=(M*M+M)/2
      M=38
      GO TO (153,154),IUD
C     DENS IS SAME AS IN BAND PROGRAM ( NOT LISTED BELOW)
  153 CALL DENS(XL,KX,KY,KZ,KMX,WT,SUM,SWUP,EN,NEN,
     1  DEN,NB1,NB2)
C     PINT OBTAINS NEW COULOMB FOURIER COEF
      CALL PINT(X1,XL,RSQ,DKUP,KNMAX,M,H,MN,WT,BZU,EF)
      GO TO 155
  154 CALL DENS(XL,KX,KY,KZ,KMX,WT,SUM,SW,EN,NEN,
     1  DEN,NB1,NB2)
      CALL PINT(X1,XL,RSQ,DKDN,KNMAX,M,H,MN,WT,BZD,EF)
  155 CONTINUE
  120 CONTINUE
      RHO=5.28
C     FERMI SAME AS IN BAND PGM. ( NOT LISTED BELOW )
      CALL FERMI(SWUP,EN,RHO,NEN,NB1,NB2,DEN,EF)
      RHO=4.72
      CALL FERMI(SW   ,EN,RHO,NEN,NB1,NB2,DEN,EF)
C     DO 156 IUD=1,1500
      DO 156 IUD=1000,3000
  156 WRITE(6,157) EN(IUD),SWUP(7,IUD),SWUP(8,IUD),
     1 SW(7,IUD),SW(8,IUD)
  157 FORMAT(1X,F13.7,10X,2F13.7,10X,2F13.7)
C     CALCULATE THE ITERATED CHARGE DENSITY COEFFICIENT
      BZ=BZU+BZD
      DO 378 KN=1,KNMAX
      DK(KN)=DKUP(KN)+DKDN(KN)
      CADS=-4.0*CON(KN) /ACONST**3/SUMW
      DK(KN)=DK(KN)*CADS
      DKUP(KN)=DKUP(KN)*CADS
      DKDN(KN)=DKDN(KN)*CADS
      II=IX(KN)**2+IY(KN)**2+IZ(KN)**2+1
      IF(KN.NE.1) GO TO 66266
C     CALCULATE RHO(0) WHICH IS NO. OF ELECTRONS IN
C     CRYSTAL/OMEGA. THEN OBTAIN NO. OF ELECTRONS
      DK(1)=DK(1)*ACONST**3/4.0
      WRITE(6,9995) DK(1)
 9995 FORMAT(1X,'RHO(0)=',E16.8)
C     BZ IS CHANGE IN K=(0,0,0) COULOMB POT. FOURIER COEF
      BZ=-16.0/3.0*CON(1)/ACONST**3*BZ/SUMW*3.14159265
     1  -VK0(1)
      WRITE(6,9967) BZ
 9967 FORMAT(1X,'DK(1)=',E16.8)
```

```
      DK(1)=BZ
      GO TO 378
66266 CONTINUE
C     ACCELERATE CONVERGENCE BE TAKING SMALL CHANGE IN RHO
      DKUP(KN)=DKUP(KN)*FACT+(1.0-FACT)*RHOOU(KN)
      DKDN(KN)=DKDN(KN)*FACT+(1.0-FACT)*RHOOD(KN)
      DK(KN)=FACT*DK(KN)+(1.-FACT)*VM(II)
  378 CONTINUE
C     XINT OBTAINS CHANGE IN EXCHANGE COEF IN XRUP AND
C     XRDN FOR NEXT ITERATION
      CALL XINT(DKUP,XRUP,CON,KNMAX,ACONST,1)
      CALL XINT(DKDN,XRDN,CON,KNMAX,ACONST,2)
      AT0=VK0(1)
      AT1=VK(1)
C     CONVERT FROM RHO(K) TO V(K)
      WRITE(6,223)
 1111 CONTINUE
      WRITE(6,32211)
32211 FORMAT(6X,'NUCLEAR',3X,'EX UP',6X,'EX DN',3X,
     1'RHOOU',3X,'RHOOD',
     *5X,'ELE',15X,'DK(KN)',13X,'DVUP',13X,'DVDN')
      DO 379 KN=1,KNMAX
      II=IX(KN)*IX(KN)+IY(KN)*IY(KN)+IZ(KN)*IZ(KN)
      K=IX(KN)
      ASQ=II
      II=II+1
      VM(II)=DK(KN)
      ASQ=ASQ*39.478418/ACONST**2
      IF(KN.EQ.1)GO TO 379
      DK(KN)=-25.132741*(DK(KN)-VK0(KN))/ASQ
      ATQ=-25.132741/ASQ*28.0*4./ACONST**3
      AT0=-25.132741/ASQ*VK0(KN)
      AT1=VK(KN)
      ATU=-25.132741/ASQ*RHOOU(KN)
      ATD=-25.132741/ASQ*RHOOD(KN)
      XRRKU=XRUP(KN)+RKUP(KN)
      XRRKD=XRDN(KN)+RKDN(KN)
  379 WRITE(6,100) IX(KN),IY(KN),IZ(KN),ATQ,VX0UP(KN),
     1 VX0(KN),ATU,ATD,AT0,AT1,DK(KN),RKUP(KN),
     2 XRUP(KN),RKDN(KN),XRDN(KN),XRRKU,XRRKD
  100 FORMAT(1X,I2,2I1,14F9.5)
      WRITE(6,223)
  223 FORMAT(1H1,'ITERATED COEFFICIENTS')
      ITER=ITER+1
      REWIND 4
      REWIND 1
      REWIND 2
      REWIND 8
      WRITE(7,236)(DK(IRLV),IRLV=1,KNMAX)
      DO 9992 I=1,KNMAX
 9992 DUM1(I)=XRUP(I)+RKUP(I)
      WRITE(7,236)(DUM1(I),I=1,KNMAX)
      DO 9991 I=1,KNMAX
```

```
 9991 DUM1(I)=XRDN(I)+RKDN(I)
      WRITE(7,236) (DUM1(I),I=1,KNMAX)
      IF(ITER.LE.NITER)GO TO 381
      WRITE(6,221)
      WRITE(6,221)
      ITER=ITER-1
      DO 9998 I=1,ITER
      WRITE(6,235)(EVAL(I,J),J=1,M)
 9998 XL(I)=EVAL(I,4)-EVAL(I,5)
      WRITE(6,221)
      DO 9997 I=1,ITER
 9997 WRITE(6,235)XL(I)
 9999 STOP
      END
      SUBROUTINE PINT(X1,XL,RSQ,RHO,KNMAX,MM,H,MN,WT,BZ,FE
C     THIS SUBROUTINE OBTAINS COULOMB POT. FOURIER COEF
      REAL *8 H,X1,XL
      DIMENSION XL(MM)
      DIMENSION X1(MM,MM),RHO(KNMAX),H(MM,MM),RSQ(MN)
      COMMON/LCS/SIJ(51,741),VK0(620),VX0(620),VM(200),
     *  SW(8,3000),EN(3000),SWUP(8,3000),RHOOU(51),
     1 RHOOD(51),VM0(800),
     1  VW(200),IX(620),IY(620),IZ(620),IMAX,KKMAX
      DO 121 IRLV=1,KNMAX
      ERO=0.
      DO 123 I=1,MM
      DO 123 J=1,I
      IJ=(I*I-I)/2+J
      H(I,J)=SIJ(IRLV,IJ)
C     IF(IRLV.EQ.1)H(I,J)=RSQ(IJ)
  123 H(J,I)=H(I,J)
      DO 125 IN=21,38
C     SUM ONLY OVER ENERGY EIGENVALUES BELOW FERMI ENERGY
      IF(XL(IN).GT.FERMIE) GO TO 125
      DO 122 I1=1,38
      DO 122 I2=1,38
  122 ERO=ERO+X1(I1,IN)*H(I1,I2)*X1(I2,IN)
  125 CONTINUE
  121 RHO(IRLV)=RHO(IRLV)+WT*ERO
      ERO=0.0
C     OBTAIN NO. OF ELECTRONS IN CRYSTAL/OMEGA FROM R**2
      DO 23 I=1,MM
      DO 23 J=1,I
      IJ=I*(I-1)/2+J
      H(I,J)=RSQ(IJ)
   23 H(J,I)=H(I,J)
      DO 25 IN=21,38
      IF(XL(IN).GT.FERMIE) GO TO 25
      DO 22 I1=1,38
      DO 22 I2=1,38
   22 ERO=ERO+X1(I1,IN)*H(I1,I2)*X1(I2,IN)
   25 CONTINUE
   21 BZ=BZ+WT*ERO
```

```
      RETURN
      END
      SUBROUTINE SORT(K,L,M)
C     THIS SUBROUTINE ASSURES K.GE.L.GE.M
      IF(L.GE.M)GO TO 401
      KK=L
      L=M
      M=KK
  401 IF(K.GE.M)GO TO 402
      KK=K
      K=L
      L=M
      M=KK
  402 IF(K.GE.L)GO TO 403
      KK=K
      K=L
      L=KK
  403 RETURN
      END
      SUBROUTINE WEIG(KA,KB,KC,KM,W)
C     COMPUTES LATTICE WEIGHTS
      KN = 3*KM/2
      IF (KA) 1,1,2
    1 W = .020833333
      GO TO 50
    2 W = 1.
      IF (KA-KM) 6,3,3
    3 W = W*.5
      KD = KA+KB+KC
      IF (KD-KN) 9,4,4
    4 W = W*.5
      GO TO 9
    6 KD = KA+KB+KC
      IF (KD-KN) 9,7,7
    7 W = W*.5
    9 IF (KC) 10,10,14
   10 W = W*.5
      IF (KB) 11,11,12
   11 W = W*.25
      GO TO 50
   12 IF (KA-KB) 13,13,50
   13 W =W*.5
      GO TO 50
   14 IF (KB-KC) 15,15,17
   15 W=W*.5
      IF (KA-KB) 16,16,50
   16 W = W*.33333333
      GO TO 50
   17 IF (KA-KB) 18,18,50
   18 W = W*.5
   50 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE XINT(VK,RK,CON,KNMAX,ACONST,NUD)
C     THIS SUBROUTINE FINDS CHANGE IN EXCHANGE COEF.
      DIMENSION VK(1),RK(1),CON(1)
      COMMON/LCS/SIJ(51,741),VK0(620),VX0(620),VM(200),
     *  SW(8,3000),EN(3000),SWUP(8,3000),RHOOU(51),
     1  RHOOD(51),VMO(800),
     1  VW(200),IX(620),IY(620),IZ(620),IMAX,KKMAX
C     SIXPI = -6.*(3/4 PI) **  1/3
      SIXPI=-6.0*(3.0/(4.0*3.14159265))**.33333333
      VOL=ACONST**3/4.
      ELEC=28.0
      C=VOL/ELEC
      DH=0.
      DO 1 KN=2,KNMAX
      I=IX(KN)
      J=IY(KN)
      K=IZ(KN)
      II=I*I+J*J+K*K+1
      GO TO (3,4),NUD
    3 DH=DH+VK(KN)**2-RHOOU(KN)**2
      GO TO 5
    4 DH=DH+VK(KN)**2-RHOOD(KN)**2
    5 CONTINUE
      RHO=0.
    2 CONTINUE
      RHO=2./3.*C*RHO
      GO TO (6,7),NUD
    6 RHO=VK(KN)-RHOOU(KN)-RHO
      GO TO 8
    7 RHO=VK(KN)-RHOOD(KN)-RHO
    8 CONTINUE
      RHO=C**.6666666*RHO/3.
      RHO=SIXPI*RHO
    1 RK(KN)=RHO
      RK(1)=-2.0/9.0*C**1.66666666*DH*SIXPI
      RETURN
      END
```

```
   2                        1.0
 1  5  81021242631333553565863656881848689
  -0.82339329E 00   0.0      0.0      0.0       4
  -0.22032099E 01   1.00     1.00     1.00      1
  -0.17206659E 01   2.00     0.0      0.0       3
  -0.95824552E 00   2.00     2.00     0.0       2
  -0.73244613E 00   3.00     1.00     1.00      1
  -0.68024045E 00   2.00     2.00     2.00      1
  -0.53128296E 00   4.00     0.0      0.0       3
  -0.45722431E 00   3.00     3.00     1.00      1
  -0.43700689E 00   4.00     2.00     0.0       2
  -0.37148803E 00   4.00     2.00     2.00      1
  -0.33400583E 00   3.00     3.00     3.00      1
```

-0.33400583E	00	5.00	1.00	1.00	1
-0.28594154E	00	4.00	4.00	0.0	2
-0.26321119E	00	5.00	3.00	1.00	1
-0.25641245E	00	6.00	0.0	0.0	3
-0.25641245E	00	4.00	4.00	2.00	1
-0.23240036E	00	6.00	2.00	0.0	2
-0.21715814E	00	5.00	3.00	3.00	1
-0.21250826E	00	6.00	2.00	2.00	1
-0.19574744E	00	4.00	4.00	4.00	1
-0.18481606E	00	5.00	5.00	1.00	1
-0.18481606E	00	7.00	1.00	1.00	1
-0.18143946E	00	6.00	4.00	0.0	2
-0.16908926E	00	6.00	4.00	2.00	1
-0.16088361E	00	7.00	3.00	1.00	1
-0.16088361E	00	5.00	5.00	3.00	1
-0.14886010E	00	8.00	0.0	0.0	3
-0.14248145E	00	7.00	3.00	3.00	1
-0.14047658E	00	8.00	2.00	0.0	2
-0.14047658E	00	6.00	4.00	4.00	1
-0.13300031E	00	8.00	2.00	2.00	1
-0.13300031E	00	6.00	6.00	0.0	2
-0.12790388E	00	7.00	5.00	1.00	1
-0.12790388E	00	5.00	5.00	5.00	1
-0.12629265E	00	6.00	6.00	2.00	1
-0.12024146E	00	8.00	4.00	0.0	2
-0.11607844E	00	7.00	5.00	3.00	1
-0.11607844E	00	9.00	1.00	1.00	1
-0.11475563E	00	8.00	4.00	2.00	1
-0.10975969E	00	6.00	6.00	4.00	1
-0.10629624E	00	9.00	3.00	1.00	1
-0.10099751E	00	8.00	4.00	4.00	1
-0.98071277E-01		9.00	3.00	3.00	1
-0.98071277E-01		7.00	7.00	1.00	1
-0.98071277E-01		7.00	5.00	5.00	1
-0.97134292E-01		8.00	6.00	0.0	2
-0.97134292E-01		10.00	0.0	0.0	3
-0.93563914E-01		10.00	2.00	0.0	2
-0.93563914E-01		8.00	6.00	2.00	1
-0.91058910E-01		7.00	7.00	3.00	1
-0.91058910E-01		9.00	5.00	1.00	1
-0.78407812E	00	0.0	0.0	0.0	4
-0.22474966E	01	1.00	1.00	1.00	1
-0.17495632E	01	2.00	0.0	0.0	3
-0.96699965E	00	2.00	2.00	0.0	2
-0.73698688E	00	3.00	1.00	1.00	1
-0.68397599E	00	2.00	2.00	2.00	1
-0.53312743E	00	4.00	0.0	0.0	3
-0.45836830E	00	3.00	3.00	1.00	1
-0.43798751E	00	4.00	2.00	0.0	2
-0.37202871E	00	4.00	2.00	2.00	1
-0.33435315E	00	3.00	3.00	3.00	1
-0.33435315E	00	5.00	1.00	1.00	1
-0.28610069E	00	4.00	4.00	0.0	2

-0.26330483E 00	5.00	3.00	1.00	1
-0.25648987E 00	6.00	0.0	0.0	3
-0.25648987E 00	4.00	4.00	2.00	1
-0.23242801E 00	6.00	2.00	0.0	2
-0.21716124E 00	5.00	3.00	3.00	1
-0.21250516E 00	6.00	2.00	2.00	1
-0.19572622E 00	4.00	4.00	4.00	1
-0.18478638E 00	5.00	5.00	1.00	1
-0.18478638E 00	7.00	1.00	1.00	1
-0.18140763E 00	6.00	4.00	0.0	2
-0.16905165E 00	6.00	4.00	2.00	1
-0.16084379E 00	7.00	3.00	1.00	1
-0.16084379E 00	5.00	5.00	3.00	1
-0.14881915E 00	8.00	0.0	0.0	3
-0.14244086E 00	7.00	3.00	3.00	1
-0.14043617E 00	8.00	2.00	0.0	2
-0.14043617E 00	6.00	4.00	4.00	1
-0.13296121E 00	8.00	2.00	2.00	1
-0.13296121E 00	6.00	6.00	0.0	2
-0.12786609E 00	7.00	5.00	1.00	1
-0.12786609E 00	5.00	5.00	5.00	1
-0.12625527E 00	6.00	6.00	2.00	1
-0.12020612E 00	8.00	4.00	0.0	2
-0.11604470E 00	7.00	5.00	3.00	1
-0.11604470E 00	9.00	1.00	1.00	1
-0.11472243E 00	8.00	4.00	2.00	1
-0.10972857E 00	6.00	6.00	4.00	1
-0.10626668E 00	9.00	3.00	1.00	1
-0.10097051E 00	8.00	4.00	4.00	1
-0.98045707E-01	9.00	3.00	3.00	1
-0.98045707E-01	7.00	7.00	1.00	1
-0.98045707E-01	7.00	5.00	5.00	1
-0.97109199E-01	8.00	6.00	0.0	2
-0.97109199E-01	10.00	0.0	0.0	3
-0.93540609E-01	10.00	2.00	0.0	2
-0.93540609E-01	8.00	6.00	2.00	1
-0.91036856E-01	7.00	7.00	3.00	1
-0.91036856E-01	9.00	5.00	1.00	1

VITA

Julius Patrick Langlinais was born on September 5, 1945 in New Iberia, Louisiana. He graduated from New Iberia High School in 1963. He received the degree of Bachelor of Science in Physics from the University of Southwestern Louisiana, Lafayette, Louisiana, in 1967. He received the degree of Master of Science from Louisiana State University, Baton Rouge, Louisiana, in 1970 in the field of Physics. He is now a candidate for the degree of Doctor of Philosophy in the Department of Physics and Astronomy.

EXAMINATION AND THESIS REPORT

Candidate: Julius Patrick Langlinais

Major Field: Physics

Title of Thesis: Energy Bands of Ferromagnetic Nickel

Approved:

Joseph Callaway
Major Professor and Chairman

Max Goodrich
Dean of the Graduate School

EXAMINING COMMITTEE:

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Date of Examination:

July 16, 1971