Band Structure of Nickel: Spin-Orbit Coupling, the Fermi Surface and Theoretical Conductivity.

Ching-ping Shih Wang
Louisiana State University and Agricultural & Mechanical College
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BAND STRUCTURE OF NICKEL: SPIN ORBIT COUPLING, 
THE FERMI SURFACE AND THE OPTICAL CONDUCTIVITY

A DISSERTATION

Submitted to the Graduate Faculty of the 
Louisiana State University and 
Agricultural and Mechanical College 
in partial fulfillment of the 
requirements for the degree of 
Doctor of Philosophy 
in 
The Department of Physics and Astronomy

by 
Ching-Ping Shih Wang
B.S., Tung-Hai University, Taiwan, 1969
M.S., Louisiana State University, Baton Rouge, La., 1971
August 1974
To My Mother
# TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>ACKNOWLEDGEMENTS</td>
<td>ii</td>
</tr>
<tr>
<td>LIST OF TABLES</td>
<td>vi</td>
</tr>
<tr>
<td>LIST OF FIGURES</td>
<td>vii</td>
</tr>
<tr>
<td>ABSTRACT</td>
<td>ix</td>
</tr>
<tr>
<td>CHAPTER I. INTRODUCTION</td>
<td>1</td>
</tr>
<tr>
<td>CHAPTER II. THE TIGHT BINDING METHOD AND SELF-CONSISTENCY PROCEDURES</td>
<td>10</td>
</tr>
<tr>
<td>A. The Basic Approximations</td>
<td>10</td>
</tr>
<tr>
<td>B. The Tight Binding Method</td>
<td>15</td>
</tr>
<tr>
<td>C. Self-Consistent Procedure</td>
<td>33</td>
</tr>
<tr>
<td>D. Spin Orbit Coupling</td>
<td>41</td>
</tr>
<tr>
<td>CHAPTER III. APPLICATIONS AND RESULTS</td>
<td>49</td>
</tr>
<tr>
<td>A. Spin and Charge Density</td>
<td>49</td>
</tr>
<tr>
<td>B. Momentum Distribution of Electrons</td>
<td>53</td>
</tr>
<tr>
<td>C. The Density of States</td>
<td>61</td>
</tr>
<tr>
<td>D. The Fermi Surface</td>
<td>64</td>
</tr>
<tr>
<td>E. Optical Conductivity</td>
<td>68</td>
</tr>
<tr>
<td>CHAPTER IV. CONCLUSION</td>
<td>80</td>
</tr>
<tr>
<td>REFERENCES</td>
<td>84</td>
</tr>
<tr>
<td>TABLES</td>
<td>93</td>
</tr>
<tr>
<td>FIGURES</td>
<td>117</td>
</tr>
<tr>
<td>APPENDICES</td>
<td>136</td>
</tr>
<tr>
<td>A. The Fourier Transform of Gaussian Orbitals</td>
<td>136</td>
</tr>
</tbody>
</table>
B. Ferromagnetic Kerr Effect 138
C. Computer Programs 142
# LIST OF FIGURES

<table>
<thead>
<tr>
<th>Figure</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>I.</td>
<td>Coordinates for the Evaluation of Three Center Integrals</td>
<td>117</td>
</tr>
<tr>
<td>II.</td>
<td>Self-Consistent Energy Bands for Majority Spin States</td>
<td>118</td>
</tr>
<tr>
<td>III.</td>
<td>Self-Consistent Energy Bands for Minority Spin States</td>
<td>119</td>
</tr>
<tr>
<td>IV.</td>
<td>Self-Consistent Energy Bands Including Spin Orbit Coupling</td>
<td>120</td>
</tr>
<tr>
<td>V.</td>
<td>Band Electrons Charge Density in Three Principle Directions</td>
<td>121</td>
</tr>
<tr>
<td>VI.</td>
<td>Magnetic Scattering Form Factors</td>
<td>122</td>
</tr>
<tr>
<td>VII.</td>
<td>Spin Density in Three Principle Directions</td>
<td>123</td>
</tr>
<tr>
<td>VIII.</td>
<td>Compton Profile in Three Principle Directions</td>
<td>124</td>
</tr>
<tr>
<td>IX.</td>
<td>Anisotropy in Compton Profile</td>
<td>125</td>
</tr>
<tr>
<td>X.</td>
<td>Comparison of the Spherical Average</td>
<td>126</td>
</tr>
<tr>
<td>XI.</td>
<td>Projected Density of States for Majority Spin</td>
<td>127</td>
</tr>
<tr>
<td>XII.</td>
<td>Projected Density of States for Minority Spin</td>
<td>128</td>
</tr>
<tr>
<td>XIII.</td>
<td>Total Density of States</td>
<td>129</td>
</tr>
</tbody>
</table>
XIV. Fermi Surface Cross Section in the (100) Plane ......................... 130
XV. Fermi Surface Cross Section in the (110) Plane ......................... 131
XVI. Joint Density of States ........................................... 132
XVII. The Real Part of the $\sigma_{xx}$ Component of the Conductivity Tensor from 0 to 1.2 eV .................. 133
XVIII. The Real Part of $\sigma_{xx}$ from 1.0 eV to 6.0 eV .................. 134
XIX. The Imaginary Part of $\sigma_{xy}$ from 0 to 6 eV .................. 135
calculated using matrix elements computed from wave functions including spin orbit coupling. Results were obtained for both the diagonal and the off diagonal elements of the conductivity tensor.
CHAPTER I
INTRODUCTION

Energy band computations for transition metals have been of continuing interest in solid state physics. These calculations are of fundamental importance in the construction of the band theory of itinerant electron magnetism.\(^1\) It is assumed that the electrons responsible for the magnetism are not localized, but instead occupy Bloch states with wave functions extending throughout the crystal. Four major items of evidence strongly support the applicability of the general picture of itinerant electron ferromagnetism to nickel. First, energy band calculations have reproduced in reasonable detail the Fermi surface determined by measurements of the de Haas-Van Alphen effect and cyclotron resonance. Second, the saturation moment for nickel is found to be \(0.616\) Bohr magnetons/atom.\(^2\) The difference from an integral number is too large to be attributed to an orbital component of the magnetic moment. Third, the high field Hall and magnetoresistance measurements of Fawcett and Reed\(^3\) indicate that the 3d electrons responsible for the magnetism have a mobility comparable with those of predominant s-p character. Fourth, the electronic specific heat measurement for nickel, \(7.028\) mJ/(mol K\(^2\)),\(^3\) shows that at least some of the 3d electrons have acquired an
Itinerant behavior and contributed to the Fermi surface. A detailed comparison of itinerant versus localized-spin models can be found in Herring's book.\(^5\)

Some of the more important calculation on the band structure of nickel used the LCAO (tight binding) method, \(^6\)-\(^{11}\) the APW (Augmented Plane Wave) method, \(^{12}\)-\(^{15}\) the KKR (Green function) method, \(^8\),\(^{16}\)-\(^{17}\) and the combined interpolation scheme. \(^{16}\),\(^{18}\)-\(^{23}\) Both APW \(^{24}\)-\(^{26}\) and KKR \(^{27}\),\(^{28}\) methods, in their usual forms, employ the "muffin-tin" approximation in which the crystal potential is assumed to be spherically symmetric in spheres inscribed within a polyhedral atomic cell about each lattice site and constant between these spheres. In the case of a APW calculation, the electronic wave functions are expanded in terms of spherical waves (products of radial wave functions and spherical harmonics) inside each sphere and plane waves between them. The eigenvalue problem is solved by varying the expansion coefficients in such a way that the logarithmic derivatives of wave functions are continuous across the boundary of the spheres. The KKR method employs a variational principle in which the Schrödinger equation is transformed into a homogeneous integral equation. The trial wave function is expanded in terms of spherical waves. The variational condition gives a set of linear homogeneous equations and the dispersion relation is obtained by solving the secular equation whose
matrix elements consists of two parts. The first part is a geometrical structure constant arising from the lattice Green function which needs to be calculated only once for each type of lattice. The second part involves the logarithmic derivatives of the trial radial wave functions evaluated on the inscribed sphere.

One essential problem in the energy band calculation is to obtain a self-consistent potential. The effects of different starting atomic configurations on the results of non-self-consistent band calculations have been illustrated in the work of Mattheiss. Both methods described here have been made self-consistent to the extent of the muffin-tin approximation. For a transition metal, the 3d states are moderately sensitive to the nonspherical part of the potential (the crystal field effects). The non-muffin-tin corrections to the band structure of paramagnetic nickel has been studied by Painter. The d bandwidth is narrowed by 0.010 Ry. and the s-d separation is reduced by 0.003 Ry. The L\textsubscript{2\textdagger} state which is important in determining the Fermi surface neck at L is shifted by +0.010 Ry. Although the order of the L\textsubscript{2\textdagger} and L\textsubscript{3}, states remains the same, this shift in energy is sufficiently large to effect detailed comparison with experiments.

Two calculations have been reported previously in which some degree of self-consistency was achieved. The first of these, by Wakoh employed the KKR method and used the
Slater average free electron exchange potential. The effect of reducing the parameter in the $X_a$ exchange potential has been illustrated in two self-consistent APW calculations by Connolly. The Kohn-Sham-Gaspar exchange potential ($a = 2/3$) was found to yield more realistic results than the full Slater exchange ($a = 1$). Spin orbit interaction was neglected in both calculations.

The combined interpolation scheme is an interpolative calculation which describes the energy bands in terms of a minimal basis set and corresponding disposable parameters. It combines a tight binding treatment for the d bands with a pseudo potential appropriate for the s-p bands. The basis functions consist of linear combination of atomic orbitals for d states and orthogonalized plane waves for the s-p bands. The orthogonality condition between the conduction s-p bands and the core states is simulated by the inclusion of the pseudo potential. There are two major interactions between the d bands and the conduction s-p bands. The first, hybridization, is included through the use of k dependent matrix elements. The second interaction, arising from the requirement of orthogonalization of basis states, can be either described in terms of k dependent form factors or included in the hybridization parameters. The parameters appearing in the Hamiltonian matrix elements are optimized to satisfy most experimental data and first principle calculations. The energies and
wave functions are obtained by diagonalizing the Hamiltonian matrix at a general point of the Brillouin zone. The $k\cdot p$ perturbation theory has been proved to be very useful to determine the energies in the vicinity of symmetric points. In general, the combined interpolation scheme provides a simple and economical way of calculating energy bands, when enough experimental information is available to determine the parameters.

The LCAO method employs the variational principle with trial Bloch functions expanded in terms of localized orbitals suitably formed at each lattice site. In its original form, this method is limited by severe problems involving calculation of three center integrals. Lin and co-workers showed that this difficulty can be avoided by expressing the crystal potential as Fourier series over the reciprocal lattice vectors. Furthermore, the Hamiltonian and overlap matrix elements can be expressed in a closed form if the basis set is chosen to consist of Gaussian type orbitals. This method has the advantage that energies and eigenfunctions can be obtained directly at a large number of points in the Brillouin zone without resorting to an interpolation scheme.

The self-consistent procedure within the framework of the tight binding approximation was first introduced by Callaway and Fry. The present work is the first self-consistent tight binding calculation ever achieved. The Hamiltonian and overlap matrix elements obtained in the
previous non-self-consistent tight binding calculation for ferromagnetic nickel by Langlinais and Callaway\textsuperscript{10} were used as input material for the first iteration of the self-consistent procedure. Eighty-nine points in $1/48$th of the Brillouin zone were used to determine the charge density in the final stages of an iterative procedure. Exchange has been included according to the Xu method.\textsuperscript{35} It was found that the Kohn-Sham-Gaspar\textsuperscript{33,34} value of the coefficient $a(2/3)$ appeared to yield the most satisfactory results for the Fermi surface and other properties. Separate exchange potentials are obtained for electrons of majority and minority ($\uparrow$ and $\downarrow$) spins and energy bands are computed separately for the two spin states. This calculation is a test of the ability of such a procedure (the spin-polarized method) to account for the magnetic and electronic properties of a ferromagnetic metal. The results obtained are in reasonable agreement with a variety of different experiments and other self-consistent calculations. This method was later applied to ferromagnetic iron,\textsuperscript{40} paramagnetic chromium,\textsuperscript{41} and potassium.\textsuperscript{42} The results are found to be equally successful.

This calculation was subsequently extended to include the effects of spin orbit coupling. Spin orbit coupling is of major significance in a description of the properties of ferromagnetic transition metals. It leads to the existence of magnetic anisotropy, the anomalous Hall effect,
and magneto-optical effects. Substantial modifications of the Fermi surface result from changes in the connectivity of the energy bands. Attempts have been made to study spin orbit effects in the band structure of nickel for more than 30 years.\textsuperscript{18,22,43-49} Much of this work, however, has been based on oversimplified tight binding models of the d band structure. Other investigations have employed interpolation schemes designed to fit empirical information concerning the band structure, magnetic properties, and Fermi surface.\textsuperscript{18,22} We are not aware of previous attempts to include spin orbit coupling into a first principles band calculation for this metal.

The plan of this dissertation is as follows: In Chapter II we outline the procedure of a self-consistent tight binding calculation including the effects of both exchange and spin-orbit coupling. Some emphasis has been placed on the basic approximations reviewed in Section A. Modifications and improvements have been included in the discussion of the tight binding method and the construction of initial one electron potential in Section B. For an exact description of the procedure to construct the non-self-consistent energy bands for nickel, one is referred to Langlinais's dissertation.\textsuperscript{10} Section C contains a detailed discussion of the self-consistent procedure. The method employed to incorporate spin orbit interaction is presented in Section D. The energy bands
obtained before and after including the effects of spin orbit interaction are discussed at the end of Sections C and D respectively.

Chapter III is designated to compare the energies and wave functions obtained with the results of different experiments. In Section A the charge and spin density are compared with the X-ray and neutron diffraction measurements. The momentum distribution of electrons was examined through the calculation of the Compton profile in Section B. The Fermi surface effects on the structure observed in the Compton profile is analyzed. Spin orbit interaction is neglected in the above calculations. Including the effects of spin orbit interaction, energies, wavefunctions, and momentum matrices were obtained at 1357 regularly spaced points in 1/16th of the Brillouin zone. The density of states discussed in Section C was obtained by the Gilat-Raubenheimer method in combination with an interpolation scheme. The Fermi surface properties are shown in Section D and are compared with experiments. Major emphasis has been placed on the calculation of the optical conductivity tensor. The one electron theory of the interband conductivity tensor is discussed in Section E. A possible lifetime broadening effect has been considered through the inclusion of a phenomenological constant relaxation time. Detailed analysis and comparison with the ordinary and magneto-optical measurements are
attempted. Our general conclusions are stated in Chapter IV. A complete set of computer programs is included in Appendix C. The first few programs concerning the construction of the initial one electron potential and the Hamiltonian matrices have been rewritten in order to improve their accuracy and efficiency. They will be used subsequently to calculate the band structure of vanadium.
CHAPTER II

THE TIGHT BINDING METHOD AND SELF-CONSISTENCY PROCEDURES

This chapter is divided into four sections. In Section A, we shall briefly discuss the basic approximations. In Section B, we shall review the tight binding method, the choice of a basis set, and the construction of a one-electron potential. In Section C, we shall outline the self-consistency procedure within the framework of tight binding approximation. In Section D, we shall describe the methods employed to incorporate the spin orbit interaction.

A. The Basic Approximations

To calculate the energy levels of electrons in solids one has to solve the Schrödinger equation for a very large number of nuclei and electrons. Numerous simplifying approximations are necessary in order to solve this many body problem. The basic approximations involved in the framework of energy band theory are: first, the solid is an infinite periodic array of atoms or ions; second, the electronic and nuclear motions are independent, the Born Oppenheimer approximation; and third, the single electron moves in a periodic potential due to the nuclei and other electrons, the Hartree-Fock theory.
It is usually not possible to solve the Hartree-Fock equation directly due to the non-local nature of the exchange potential. Several approximations have been developed to construct an averaged local exchange potential. We shall briefly outline them here:

The first approximation was introduced by Slater and is based on the theory of the free electron gas. The exchange potential in a gas of density \( \rho \) is given by

\[ v_{\text{gas}} = -8 F\left(\frac{|\mathbf{k}|}{k_F}\right) \left(\frac{3}{8\pi} \rho\right)^{1/3} \tag{2.1} \]

where \( \mathbf{k} \) is the wave vector of a plane wave state. Electrons occupy states within a sphere centered on \( \mathbf{k}=0 \) and of radius \( k_F \) for each spin, with

\[ F(y) = \frac{1}{2} + \frac{1-y}{4y} \ln \left| \frac{1+y}{1-y} \right| . \tag{2.2} \]

Atomic units are used throughout this paper unless otherwise specified. In the Hartree Fock theory the density of states, which depends inversely on \( dE/dk \), would vanish on the Fermi surface. This is one of the major difficulties of Hartree-Fock theory, which results from the neglect of electron correlation. It can be avoided if one considers an averaged local exchange potential. The simplest approximation is to treat \( \rho \) as the local charge density and to replace \( F(y) \) by its average value over all
occupied states, 3/4. Thus we have an exchange potential which we call $V_{xS'}$

$$V_{xS} = -6 \left[ \frac{3}{8\pi} \rho(r) \right]^{1/3}.$$  \hspace{1cm} (2.3)

An alternative approximation to the exchange potential was suggested by Kohn and Sham$^{33}$ following an earlier treatment by Gaspar.$^{34}$ They applied the variational method to an inhomogeneous system of interacting electrons. In the limit of slowly varying density this procedure leads to an exchange potential differing from $V_{xS}$ in that the value of $F(y)$ at the Fermi level, namely 1/2 is used.

$$V_{x,KSG} = -4 \left[ \frac{3}{8\pi} \rho(r) \right]^{1/3} = \frac{2}{3} V_{xS}.$$  \hspace{1cm} (2.4)

Attempts have been made to use an exchange potential

$$V_{x\alpha} = \alpha V_{xS}$$  \hspace{1cm} (2.5)

now known as the $x\alpha$ method. The parameter $\alpha$ is allowed to vary between 1 and 2/3 or even slightly smaller than 2/3 to get the best result.

It may seem desirable to choose the value of $\alpha$ which minimizes the total energy of the system since the theory is based on the variational approximation. The objection against this procedure is that the Hamiltonian instead of
the wavefunctions is varied in the process. Our calculation employed this $X\alpha$ exchange potential. The parameter $\alpha$ is chosen to yield the best results in comparison with experimental measurements. It will be discussed in more detail in Section C.

A more elaborate suggestion was made by Liberman,$^{50}$ independently of Sham and Kohn,$^{51}$ and later modified by Slater, Wilson and Wood$^{35}$ to retain the dependence of $F(y)$ on $y$ with $y=k/k_F$ determined in the free electron gas approximation as a function of energy and density. The problem can be solved self-consistently but the cost in computer time is very high. For a more detailed discussion and comparison of exchange potentials one is referred to the paper by Slater, Wilson and Wood.$^{35}$ A generalization of the Kohn-Sham theory of the inhomogeneous electron gas with emphasis on spin effects was later made by Rajagopal and Callaway.$^{52}$ For a ferromagnetic system the exchange potential can be written as:

$$ u \ V_{X\alpha}(r) = -6u \left[ \frac{3\rho_\sigma(r)}{4\pi} \right]^{1/3} \quad (2.6) $$

where $u=\uparrow, \downarrow$ and $\rho_\sigma(r)$ is the density of electron with spin $\sigma$.

We consider the following one-electron Hamiltonian

$$ H_{\alpha} = -\nabla^2 + V_C(r) + u \ V_X(r) + V_{SO}(r) \quad (2.7) $$
The first term is the kinetic energy. The second term is the Coulomb potential which can be represented by the superposition of atomic potential at each lattice sites.

$$V_c(\mathbf{r}) = \sum_{\mu} V_a(\mathbf{r} - \mathbf{R}_\mu).$$  \hspace{1cm} (2.8)

The atomic potential due to the nuclei and the electron charge distribution $\rho_a(r)$ can be expressed as

$$V_a(\mathbf{r}) = -\frac{2Z}{|\mathbf{r}|} + 2 \int \frac{\rho_a(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3r'$$  \hspace{1cm} (2.9)

where $Z$ is the atomic number which is 28 for nickel. The third term in Eq. (2.7) is the Xα exchange potential for a spin polarized system as shown in Eq. (2.6) and the last term is the spin-orbit interaction.

$$V_{SO}(\mathbf{r}) = -\frac{\hbar}{2m^*cZ} [\mathbf{\hat{\sigma}} \times \mathbf{V}(\mathbf{r})] \cdot \hat{\mathbf{P}},$$  \hspace{1cm} (2.10)

where $\mathbf{\hat{\sigma}}$ is the Pauli spin operator, $\mathbf{V}(\mathbf{r})$ is the crystal potential and $\hat{\mathbf{P}}$ is the momentum operator. The last term was neglected in this calculation until the self-consistent procedure had been completed. It will be discussed in detail in Section D.
B. The Tight Binding Method

The tight binding or LCAO (Linear Combination of Atomic Orbitals) method was first proposed by Bloch (1928) and later modified by Lafon and Lin (1966). The three center integrals which are normally encountered in the tight binding calculations can be eliminated by expressing the crystal potential as Fourier series over the reciprocal lattice vectors. If the basis set is chosen to consist of Gaussian type orbitals (GTO) all integrals can be done analytically. The elements of the Hamiltonian and overlap matrices are expressed analytically in terms of the inter-atomic distance and Gaussian exponent parameters. A drastic reduction in the computation can therefore be effected.

In a LCAO calculation, one begins with a set of localized functions \( u_j(\mathbf{r}) \) which for convenience will be assumed to be normalized but need not be orthogonal. Conventionally \( u_j(\mathbf{r}) \) are chosen to be the atomic orbitals of the corresponding crystal. However, this is not necessary and may even be too restrictive. In the present calculation we used atomic wave functions (GTO) for all states except 3d (e.g. 1s, 2s, 3s, 4s, 2p, 3p, and 4p). The Gaussian exponent parameters and expansion coefficients were determined by Wachters from a self-consistent field calculation of free nickel atom. We believe it is
necessary to give the d wave functions more freedom to distort in the crystalline environment. A set of five separate radial GTO were used for each type of angular dependence. The orbital exponents used in defining these d functions were the same as given by Wachters.\textsuperscript{53} The basis set thus consisted of 38 functions for each spin: 4 for s-type symmetry (1s, 2s, 3s, and 4s), 9 for p-type symmetry (2p\textsubscript{x}, 2p\textsubscript{y}, 2p\textsubscript{z}, 3p\textsubscript{x}, 3p\textsubscript{y}, 3p\textsubscript{z}, 4p\textsubscript{x}, 4p\textsubscript{y}, and 4p\textsubscript{z}), and 25 for d-type symmetry (xy, yz, zx, x\textsuperscript{2}-y\textsuperscript{2}, and 3z\textsuperscript{2}-r\textsuperscript{2}).

The use of GTO has been criticized since these functions have zero slope at the origin and decay too fast at large distances. In a crystal the second problem may not be as serious as in the case of a free atom since its long distance behavior is strongly modified by the overlap of wave functions on the neighboring lattice sites. To investigate the first problem we compared the Hartree-Fock atomic wave functions based on GTO\textsuperscript{53} with those based on STO (Slater-type orbitals).\textsuperscript{54} At the origin they disagree by about 2%. Therefore our charge density at the nuclei sites had an uncertainty of about 4% resulting from the use of GTO.

The basis function ψ\textsubscript{j}(\mathbf{k}, \mathbf{r}) which satisfies Bloch's theorem for wave vector \mathbf{k} can be written as

\[ \psi\textsubscript{j}(\mathbf{k}, \mathbf{r}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}} e^{i \mathbf{k} \cdot \mathbf{R}} u\textsubscript{j}(\mathbf{r} - \mathbf{R}) \] \hspace{1cm} (2.11)
where $N$ is the total number of atoms in the crystal. The localized orbitals $u_j(r-R_{\mu})$ are centered at lattice site $R_{\mu}$. The crystal structure for nickel is face centered cubic. Its lattice constant is 6.644 a.u. when extrapolated to 0°K using the coefficient of thermal expansion.\(^{55}\)

The localized orbitals can be separated into radial and angular parts

$$u_j(r) = u_{n\ell m}(r) = \mathbf{R}_n\mathbf{K}_{\ell m}(\theta, \phi) \quad (2.12)$$

where $\mathbf{K}_{\ell m}(\theta, \phi)$ are the Kubic harmonics and the radial wavefunction can be represented by GTO

$$\mathbf{R}_n\mathbf{K}_\ell(r) = \mathbf{N}_{\ell i} r^{\ell-1} e^{-\alpha_{\ell i} r^2} \quad (2.13)$$

with the normalization constant given as

$$N_{\ell i} = \frac{2(2 \alpha_{\ell i})^{\ell+1/2}}{\Gamma(\ell + \frac{1}{2})} \frac{1}{1/2} \quad (2.14)$$

In the cases where atomic wavefunctions were required the $\mathbf{R}_n\mathbf{K}_\ell(r)$ were linearly expanded in GTO

$$\mathbf{R}_n\mathbf{K}_\ell(r) = \sum_i C_{n\ell i} N_{\ell i} r^{\ell-1} e^{-\alpha_{\ell i} r^2} \quad (2.15)$$

where we have included the principle quantum number $n$.

The values $C_{n\ell i}$ and $\alpha_{\ell i}$ have been tabulated by Wachters.\(^{53}\)
In the modified LCAO calculation the crystal potential is expanded in Fourier series

$$V(\mathbf{r}) = \sum_{\mathbf{K}} e^{i\mathbf{K} \cdot \mathbf{r}} V(\mathbf{K})$$  \hspace{1cm} (2.16)

which can be inverted to obtain

$$V(\mathbf{K}) = \frac{1}{N\Omega} \int \frac{e^{-i\mathbf{K} \cdot \mathbf{r}}}{\mathbf{r}} V(\mathbf{r}) \, d^3 \mathbf{r}$$  \hspace{1cm} (2.17)

with $\Omega$ being the volume of a primitive cell. For a periodic potential, $V(\mathbf{K})$ vanishes unless $\mathbf{K}$ is a reciprocal lattice vector. The Coulomb part of the potential has been discussed in Section A. It was assumed that for the initial iterative stage of the self-consistent calculation the crystal charge density can be represented by the superposition of overlapping neutral atom charge density, the atoms being in $3d^94s^1$ configuration. This is somewhat different from the ground state configuration of a free nickel atom ($3d^84s^2$) because the effective occupation number is expected to change in forming a crystal as the sharp atomic energy levels broaden into overlapping bands. The starting electronic configuration should in principle be immaterial to a self-consistent calculation.

The magneton number which is the difference of occupation number between up and down spin has been measured to be 0.56 electrons per atom.\(^2\) We assume in
the first iteration that this is due to d electrons only. The spherically averaged atomic charge density in Eq. (2.9) can be written as

\[ \rho_a(r) = \rho_{a1}(r) + \rho_{a2}(r) \]  

(2.18)

with

\[ \rho_{a2}(r) = \frac{1}{4\pi} \sum_i n_{i0} |R_i(r)|^2 . \]  

(2.19)

We use the radial wavefunction obtained by Clementi (1965) in a Hartree-Fock self-consistent field calculation for free nickel atom in 3d^4s^2 configuration in constructing the initial charge densities. The occupation numbers assumed are as follows:

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<th>(i)</th>
<th>1s</th>
<th>2s</th>
<th>2p</th>
<th>3s</th>
<th>3p</th>
<th>4s</th>
<th>3d</th>
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<td>(n_{i\uparrow})</td>
<td>1</td>
<td>1</td>
<td>3</td>
<td>1</td>
<td>3</td>
<td>0.5</td>
<td>4.78</td>
</tr>
<tr>
<td>(n_{i\downarrow})</td>
<td>1</td>
<td>1</td>
<td>3</td>
<td>1</td>
<td>3</td>
<td>0.5</td>
<td>4.22</td>
</tr>
</tbody>
</table>

The Fourier coefficient of the Coulomb potential is

\[ V_c(\mathbf{k}) = \frac{1}{N_{\uparrow\downarrow}} \int \frac{d^3 r}{2\pi} \frac{e^{-i\mathbf{k} \cdot \mathbf{r}}}{N_{\uparrow\downarrow}} \left[ V_c(\mathbf{r}) - V_d(\mathbf{r}) \right] d^3 r \]

\[ = \frac{1}{N_{\uparrow\downarrow}} \int \frac{d^3 r}{2\pi} \frac{e^{-i\mathbf{k} \cdot \mathbf{r}}}{N_{\uparrow\downarrow}} \left[ -i\mathbf{k} \cdot \hat{\mathbf{R}} \right] \left[ \sum_{\mu} e^{-i\mathbf{k} \cdot \mathbf{R}_\mu} V_d(\mathbf{r}) d^3 r \right] \]

\[ = \frac{1}{N_{\uparrow\downarrow}} \int \frac{d^3 r}{2\pi} \frac{e^{-i\mathbf{k} \cdot \mathbf{r}}}{N_{\uparrow\downarrow}} \left[ -i\mathbf{k} \cdot \hat{\mathbf{R}} \right] V_d(\mathbf{r}) d^3 r . \]  

(2.20)
Using the relation

\[ \frac{-i \mathbf{K} \cdot \mathbf{R}}{R} \delta_{\mathbf{K}_s \mathbf{K}_s} = N \delta_{\mathbf{K}_s \mathbf{K}_s} \]  \tag{2.21}

where \( \mathbf{K}_s \) is a reciprocal lattice vector. We obtain

\[ V_c(\mathbf{K}_s) = \frac{1}{2\pi} \int V_a(\mathbf{r}) e^{-i \mathbf{K}_s \cdot \mathbf{r}} d^3 \mathbf{r}. \]  \tag{2.22}

Eq. (2.9) is substituted into Eq. (2.22). One obtains

\[ V_c(\mathbf{K}_s) = -\frac{8\pi Z}{\varepsilon K_s^2} + \frac{32\pi^2}{\varepsilon K_s^3} \int_0^\infty \nu_a(\mathbf{r}) \sin(K_s r) r dr. \]  \tag{2.23}

With \( \nu_a(\mathbf{r}) \) given in Eq. (2.18) the integral can be easily evaluated.

For the limit \( \mathbf{K}_s \to 0 \) one has to expand the sine term in the integrand before taking the limit \( \mathbf{K}_s \to 0 \)

\[ V_c(0) = \lim_{K_s \to 0} \left[ -\frac{8\pi Z}{\varepsilon K_s^2} + \frac{32\pi^2}{\varepsilon K_s^3} \int_0^\infty \nu_a(\mathbf{r}) \sin(K_s r) r dr \right. \]

\[ \left. + \frac{(K_s r)^3}{3!} + \ldots \right] r dr \]

\[ = \lim_{K_s \to 0} \left[ -\frac{8\pi Z}{\varepsilon K_s^2} + \frac{8\pi Z}{\varepsilon K_s^2} \int_0^\infty \nu_a(\mathbf{r}) r^4 dr - \frac{16\pi^2}{3\varepsilon} \int_0^\infty \nu_a(\mathbf{r}) r^4 dr \right] \]

\[ = -\frac{16\pi^2}{3\varepsilon} \int_0^\infty \nu_a(\mathbf{r}) r^4 dr \]  \tag{2.24}
which can be readily evaluated analytically. The construction of an averaged local exchange potential has been discussed in Section A. The corresponding Fourier coefficients for spin $\sigma$ are

$$V_{\chi \sigma}(\mathbf{k}) = \frac{1}{N} \int e^{-i\mathbf{k} \cdot \mathbf{r}} V_{\chi \sigma}(\mathbf{r}) d^3r$$

$$= \frac{1}{N} \int_{\text{cell}} e^{-i\mathbf{k} \cdot \mathbf{r}} V_{\chi \sigma}(\mathbf{r}) d^3r$$

$$= \frac{4\pi}{N_{k}} \int_{0}^{r_{0}} 6 \left( \frac{3}{4\pi} \rho_{\sigma}(\mathbf{r}) \right)^{1/3} \sin(K_{s}r) rd r$$

(2.25)

where $r_{0}$ is the radius of the Wigner-Sitz sphere which has a volume equal to that of a primitive cell. The spherical averaged total charge density for electrons of spin $\sigma$ can be written as

$$\rho_{\sigma}(\mathbf{r}) = \langle \mathbf{r} \mid \rho_{\sigma}(\mathbf{r}) \mid \mathbf{r} \rangle_{av}$$

(2.26)

where the atomic charge density $\rho_{\sigma}(\mathbf{r})$ is defined in Eq. (2.19). The summation from each lattice site was carried out up to the shell of neighbors where the desired degree of convergence has been reached. Although the individual atomic charge densities were assumed to be spherically symmetric, the superposed density has only cubic
symmetry about any lattice site. The bracket \( \langle \cdots \rangle_{av.} \) stands for the spherical average evaluated in the following way: The total charge density is expanded in a series of cubic harmonics up to the eighth order. The spherical average \( \rho_{av}(r) \) is approximated as the zeroth order term in the expansion, and can be obtained by solving a set of four linear inhomogeneous equations along four inequivalent directions. Finally, the 96 point Gaussian formula was used to perform the numerical integration in the Wigner-Sitz sphere for each given reciprocal lattice vectors.

The one-electron Schrödinger equation to be solved takes the following form

\[
\hat{H} \psi_n(\mathbf{k}, \mathbf{r}) = E_n(\mathbf{k}) \psi_n(\mathbf{k}, \mathbf{r})
\]  

(2.27)

where \( \hat{H} \) is the Hamiltonian described in Eq. (2.7). The crystal wavefunction \( \psi_n(\mathbf{k}, \mathbf{r}) \) were expanded as a series in the basis function \( \phi_i(\mathbf{k}, \mathbf{r}) \)

\[
\psi_n(\mathbf{k}, \mathbf{r}) = \sum_i a_{ni}(\mathbf{k}) \phi_i(\mathbf{k}, \mathbf{r})
\]  

(2.28)

in which \( n \) is the band index and \( \mathbf{k} \) is the wave vector of the state. The set of basis functions consisting of only atomic states does not form a complete set, so the corresponding eigenfunctions are not the exact solution of the Schrödinger equation. However, inclusion of all the
bound states and some of the excited states can be expected to yield a fair approximation to the actual wavefunctions. The expansion coefficient $a_n(\vec{k})$ and energy $E_n(\vec{k})$ are to be determined by solving the Secular equation

$$\text{Det}\left|H_{mn}(\vec{k})-\varepsilon S_{mn}(\vec{k})\right|=0 \quad (2.29)$$

where

$$H_{mn}(\vec{k}) = \langle \phi_m(\vec{k},\vec{r})|\hat{H}|\phi_n(\vec{k},\vec{r})\rangle$$

$$= \frac{1}{R_m} \int u^*_m(\vec{r}-\vec{R}_\mu)\hat{H}u_n(\vec{r}) \, d^3r$$

$$= T_{mn}(\vec{k}) + V_{mn}(\vec{k}) \quad (2.30)$$

The kinetic energy matrix is given by

$$T_{mn}(\vec{k}) = \frac{1}{R_m} \int u^*_m(\vec{r}-\vec{R}_\mu)(-\nabla^2)u_n(\vec{r}) \, d^3r$$

$$\quad . \quad (2.31)$$

The matrix element of the crystal potential expanded in Fourier series over the reciprocal lattice vectors can be expressed as follows
\[ V_{mn}(k) = \frac{1}{K_S} \left[ V_C(K_S) + aV_{XO}(K_S) \right] S_{mn}(k,K_S). \] 

(2.32)

The generalized overlap matrix is given by

\[ S_{mn}(k,K_S) = \frac{1}{R_{\mu}} \left[ e^{-i(k-r)\cdot R_{\mu}} \int u_m^*(r-R_{\mu}) e^{i\hat{K}_S\cdot r} u_n(r) \right] \] 

(2.33)

For a crystal with inversion symmetry the \( e^{i\hat{K}_S\cdot r} \) term in the above equation can be replaced by \( \cos (\hat{K}_S\cdot r) \). The overlap matrix element in Eq. (2.29) is

\[ S_{mn}(k) = S_{mn}(k,\hat{0}) \] 

(2.34)

All these matrix elements can be evaluated analytically provided one choose linear combinations of GTO as the basis functions. No method has yet been found to express them in a closed form when the atomic wave functions are expanded in Slater-type orbitals. This was the reason for choosing GTO in the expansion of the basis function. We shall evaluate the integral \( \langle u_{k,m,n}(\hat{r}_A) | \cos \hat{K}\cdot \hat{r} | u_{q,s,t}(\hat{r}_B) \rangle \) following the procedure modified by Chaney and Dorman. The function \( u_{q,mn}(\hat{r}) \) are GTO of order \((k,m,n)\)
Appropriate normalization constants for both the orbital and the angular parts of the wavefunctions have to be included. The orbital on the left hand side has exponent $\alpha_1$ and is centered at lattice site $\hat{A}$ and that on the right hand side has exponent $\alpha_2$ and is centered at $\hat{B}$. The coordinates for various points are shown in Fig. 1. The integral appearing in Eq. (2.33) can be obtained by putting $\hat{B}$ and $\hat{C}$ at the origin.

\[
\langle \hat{v}, \ell, m, n (\hat{r} \mathbf{A}) | \cos \hat{k} \cdot \hat{r} \mathbf{C} | \hat{u}_{q, s, t} (\hat{r} \mathbf{B}) \rangle
\]

\[
= \int d^3 \mathbf{r} \cdot x_{\hat{A}}^\ell y_{\hat{A}} m z_{\hat{A}} n e^{-\alpha_1 \mathbf{r}^2} \cos \hat{k} \cdot \hat{r} \mathbf{C} \cdot x_{\hat{B}} q y_{\hat{B}} s z_{\hat{B}} t e^{-\alpha_2 \mathbf{r}^2} \quad (2.36)
\]

where

\[
\hat{r} \mathbf{A} = \hat{r} - \hat{A}, \quad \hat{r} \mathbf{B} = \hat{r} - \hat{B} \quad \text{and} \quad \hat{r} \mathbf{C} = \hat{r} - \hat{C}.
\]

The product of two Gaussians situated at center $\hat{A}$ and $\hat{B}$ is proportional to a third Gaussian situated at a point $\hat{D}$ along the line $\overline{AB}$

\[
\exp(-\alpha_1 \mathbf{r}_A^2 - \alpha_2 \mathbf{r}_B^2) = \exp\left(- \frac{\alpha_1 \alpha_2}{\alpha_1 + \alpha_2} \mathbf{r}_D^2\right) \exp\left(- (\alpha_1 + \alpha_2) \mathbf{r}_D^2\right) \quad (2.37)
\]

where
\[ \vec{D} = \frac{\alpha_1 \vec{A} + \alpha_2 \vec{B}}{\alpha_1 + \alpha_2} \]  
(2.38)

and

\[ \overrightarrow{AB} = \hat{B} - \hat{A} \]  
(2.39)

Writing

\[ \vec{r}_A = \vec{r}_D + \overrightarrow{AD}, \quad \vec{r}_B = \vec{r}_D + \overrightarrow{BD} \]  
and \[ \vec{r}_C = \vec{r}_C + \overrightarrow{CD} \]  
(2.40)

and taking the binomial expansion, the integral can be written as

\[ \int \left( \overrightarrow{AD}^a \overrightarrow{B}^b \overrightarrow{C}^c \overrightarrow{D}^d \overrightarrow{E}^e \overrightarrow{F}^f \right) \]  
\[ \times (\overrightarrow{BD})^{q-d} (\overrightarrow{BD})^{s-e} (\overrightarrow{BD})^{t-f} \]

\[ \left[ \cos \hat{k} \cdot \overrightarrow{CD} \cdot u_{a,b,c} (\vec{r}_D) \right] \cos \hat{k} \cdot \vec{r}_D \left| u_{d,e,f} (\vec{r}_D) \right| \]

\[ - \sin \hat{k} \cdot \overrightarrow{CD} \cdot u_{a,b,c} (\vec{r}_D) \sin \hat{k} \cdot \vec{r}_D \left| u_{d,e,f} (\vec{r}_D) \right| \]

(2.41)
where

\[ \hat{c} = \exp \left[ -\frac{\alpha_1 \alpha_2}{\alpha_1 + \alpha_2} \hat{A} B^2 \right] \quad (2.42) \]

and \( \binom{\ell}{a} \) are binomial coefficients with \( 0 \leq a \leq \ell \). The remaining integrals are central cell integrals about lattice site \( \vec{b} \). These can be evaluated analytically in Cartesian coordinates. For a crystal with inversion symmetry only those terms which are even functions of \( K_x, K_y, \) and \( K_z \) will contribute. The integral can be reduced to

\[ \ldots \]

\[ \frac{(-1)^{a+b+c+d+e+f}}{G_{a+d}(K_x, CD_x) G_{b+e}(K_y, CD_y) G_{c+f}(K_z, CD_z)} \quad (2.43) \]

In the case that \( n \) is an even number

\[ G_n(K, R) = \frac{(-1)^{n/2}}{2^n} (\pi \gamma)^{1/2} \exp \left( -\frac{\gamma K^2}{4} \right) H_n \left( \frac{K}{2}, \gamma \right) \cos(KR) \quad (2.44) \]

where
\[
\gamma = \frac{1}{\alpha_1 + \alpha_2} \quad (2.45)
\]

\(H_n^{(K, \gamma)}\) is a Hermite polynomial satisfying the following recurrence relation

\[
H_{n+2}(\frac{K}{2}, \gamma) = K\gamma H_{n+1}(\frac{K}{2}, \gamma) - 2(n+1)\gamma H_n(\frac{K}{2}, \gamma) \quad (2.46a)
\]

with

\[
H_0(\frac{K}{2}, \gamma) = 1 \quad (2.46b)
\]

and

\[
H_1(\frac{K}{2}, \gamma) = K\gamma \quad (2.46c)
\]

In the case in which \(n\) is an odd number,

\[
G_n(K, R) = K[\frac{n}{2} + 1)]^{\frac{n+1}{2}} \binom{\frac{n+1}{2}}{1} _1F_1\left(\frac{n}{2} + 1, \frac{3}{2}; -\frac{\gamma K^2}{4}\right)
\]

\[
(2.47)
\]

where \(\Gamma\left(\frac{n}{2} + 1\right)\) is the Gamma function and \(1_F_1\left(\frac{n}{2} + 1, \frac{3}{2}; -\frac{\gamma K^2}{4}\right)\) is a confluent hypergeometric function satisfying the following relation
\[
\frac{n}{2} \, _1F_1 \left( \frac{n}{2} + 1, \frac{3}{2}; x \right) + \left( \frac{3}{2} - n - x \right) \frac{n}{2} \, _1F_1 \left( \frac{n}{2}, \frac{3}{2}; x \right) \\
+ \left( \frac{n}{2} - \frac{3}{2} \right) \frac{n}{2} \, _1F_1 \left( \frac{n}{2} - 1, \frac{3}{2}; x \right) = 0
\] (2.48a)

with

\[
\frac{n}{2} \, _1F_1 \left( \frac{3}{2}, \frac{3}{2}; x \right) = e^x
\] (2.48b)

and

\[
\frac{n}{2} \, _1F_1 \left( \frac{5}{2}, \frac{3}{2}; x \right) = \left( 1 + \frac{2}{3} x \right) e^x
\] (2.48c)

The overlap matrix element can easily be obtained by setting \( \hat{K} = 0 \). The gradient and kinetic energy matrix elements can be expressed as linear combinations of overlap matrix elements in the following way

\[
\langle u_{\nu, m, n}(\mathbf{r}_A) | V | u_{\xi, s, t}(\mathbf{r}_B) \rangle \\
= u_{\nu, m, n}(\mathbf{r}_A) | u_{\xi-1, s, t}(\mathbf{r}_B) | - 2 \langle u_{\nu, m, n}(\mathbf{r}_A) | u_{\xi+1, s, t}(\mathbf{r}_B) \rangle
\] (2.49a)

and
\[ \langle u, m, n (r_A) | -\frac{y^2}{x} | u, q, s, t (r_B) \rangle \]

\[ = -q(q-1) \langle u, m, n (r_A) | u_{q-2}, s, t (r_B) \rangle + 2u_2(2q+1) \langle u, m, n (r_A) | u, q, s, t (r_B) \rangle \]

\[ - 4u_2^2 \langle u, m, n (r_A) | u_{q+2}, s, t (r_B) \rangle \]

(2.50)

Similar expression can be obtained for the \( y \) and \( z \) components.

The Hamiltonian and overlap matrix elements are either real or imaginary depending on the parity of the wavefunction. We label them as follows

\[ H = \begin{bmatrix} \text{d} & \text{s} & \text{p} \\ \text{d} & I_{dd} \cos(k \cdot \hat{R}_\mu) & I_{sd} \cos(k \cdot \hat{R}_\mu) & i I_{pd} \sin(k \cdot \hat{R}_\mu) \\ \text{s} & I_{sd} \cos(k \cdot \hat{R}_\mu) & I_{ss} \cos(k \cdot \hat{R}_\mu) & i I_{ps} \sin(k \cdot \hat{R}_\mu) \\ \text{p} & -i I_{pd} \sin(k \cdot \hat{R}_\mu) & -i I_{ps} \sin(k \cdot \hat{R}_\mu) & I_{pp} \cos(k \cdot \hat{R}_\mu) \end{bmatrix} \]

(2.51)

where
Consider the unitary transformation $H' = U H U^{-1}$ with

$$U = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & i \end{pmatrix}$$

(2.53)

The result is

$$H' = \sum_{\mathbf{R}_\mu} \begin{pmatrix} I_{dd} \cos(k \cdot \mathbf{R}_\mu) & I_{sd} \cos(k \cdot \mathbf{R}_\mu) & I_{pd} \sin(k \cdot \mathbf{R}_\mu) \\ I_{sd} \cos(k \cdot \mathbf{R}_\mu) & I_{ss} \cos(k \cdot \mathbf{R}_\mu) & I_{ps} \sin(k \cdot \mathbf{R}_\mu) \\ I_{pd} \sin(k \cdot \mathbf{R}_\mu) & I_{ps} \sin(k \cdot \mathbf{R}_\mu) & I_{pp} \cos(k \cdot \mathbf{R}_\mu) \end{pmatrix}$$

(2.54)

Here $H'$ is real and symmetric but the $pd$ and $ps$ block must be evaluated with care to avoid a possible error of negative sign. The eigenvectors of the transformed secular equation are

$$a'_{ni}(k) = \sum_{m} U_{nm} a_{mi}(k)$$

(2.55)

The momentum matrix elements between the cell periodic part of the wavefunctions $\psi_n(k,\mathbf{r}) = e^{-i k \cdot \mathbf{r}} \psi_n(k,\mathbf{r})$ (the crystal momentum representation) are defined as
\[ p_{nm}(k) = \hat{M}_{nm}(k) + \mathcal{M} k \delta_{nm} \]  

(2.56)

in which the momentum matrix elements between the crystal wavefunctions \( \hat{M}_{nm}(k) \) can be evaluated in a similar way

\[ \hat{M}_{nm}(k) = \sum_{ij} a_{ni}(k) \hat{p}_{ij}(k) a_{mj}(k) \]

\[ = \sum_{ij} (U^{-1} a'(k))^* \hat{p}_{ij}(k) (U^{-1} a'(k))_{mj} \]

\[ = \sum_{ij} a_{ni}(k)^* (U \hat{p}(k) U^{-1})_{ij} a_{mj}(k) \]

(2.57)

where

\[
\begin{pmatrix}
d & s & p \\
-d & -\dd \sin(k \cdot \hat{R}_{\mu}) & -\sd \sin(k \cdot \hat{R}_{\mu}) & \pd \cos(k \cdot \hat{R}_{\mu}) \\
-s & \sd \sin(k \cdot \hat{R}_{\mu}) & -\ss \sin(k \cdot \hat{R}_{\mu}) & \ps \cos(k \cdot \hat{R}_{\mu}) \\
p & -\pd \cos(k \cdot \hat{R}_{\mu}) & -\ps \cos(k \cdot \hat{R}_{\mu}) & \pp \sin(k \cdot \hat{R}_{\mu})
\end{pmatrix}
\]

(2.58)

The gradient matrix elements

\[
\hat{v}_{nm} = \cdot u_n(r-R_{\mu}) |\hat{v}| u_m(r) >
\]

(2.49b)

are given in Eq. (2.49a).
In the next section we shall discuss the self-consistency procedure and the choice of the exchange parameter $\alpha$.

C. Self-Consistent Procedure

In this section we shall outline the essential feature of the self-consistency procedure. This is accomplished by an iterative method. At any given iteration a potential was constructed from the band wavefunctions calculated in the previous iteration. The new potential was again used to calculate a new set of wavefunctions. The procedure was repeated until the desired degree of convergence was achieved.

The fundamental problem is to determine a new (or iterated) potential after a given stage of band structure has been completed. Since the calculation requires only the Fourier coefficients of the potential it suffices to obtain these. It was observed that only the Fourier coefficients of the potential for a few of the shortest reciprocal lattice vectors need to be considered in the iterative procedure to achieve self-consistency. Higher coefficients describe the charge density deep inside the core of an atom and do not change appreciably. For $\mathbf{k} \neq 0$ the Fourier coefficients of the Coulomb potential can be expressed as $\ldots$
The Fourier coefficients of the electron density are given by

\[ \rho(K_s) = \frac{1}{N_\Omega} \int \rho(\mathbf{r}) e^{-iK_s \cdot \mathbf{r}} d^3r \]  

in which the charge density can be written as

\[ \rho(\mathbf{r}) = \sum_{n,k} |\psi_n(\mathbf{r})|^2. \]  

The Bloch function \( \psi_n(\mathbf{r}) \) are defined in Eq. (2.28). The summation includes that portion of the Brillouin zone in which band \( n \) is occupied. Substituting Eq. (2.61) into Eq. (2.60) and converting the sum on \( \mathbf{k} \) into an integral one obtains

\[ \rho(K_s) = \frac{1}{(2\pi)^3} \sum_{n} \sum_{i,j} \int d^3k a_{ni}^*(\mathbf{k}) S_{ij}(\mathbf{k},K_s) \]

occupied

\[ a_{nj}(\mathbf{k}) \]  

occupied

The generalized overlap matrix \( S_{ij}(\mathbf{k},K_s) \) has been defined in Eq. (2.33). In the case \( K_s = 0 \) the Fourier coefficient of the Coulomb potential must be determined by a limiting process.
This limit exists and can be obtained by expanding the exponential term in powers of $|\mathbf{k}|$ before taking the limit $\mathbf{k} \to 0$. The result is

$$V(0) = \lim_{\mathbf{k} \to 0} \left[ -\frac{8\pi Z}{\Omega k^2} + \frac{8\pi}{2N\Omega} \int e^{-i\mathbf{k} \cdot \mathbf{r}} \rho(r) \, d^3r \right]$$

(2.63)

The integral is over the volume of a primitive cell. The charge in $V(0)$ at a given stage of iteration can be evaluated analytically if we make the following assumption: first, the integral over a primitive cell can be replaced by that over the Wigner-Sitz sphere, and second, the change in $\rho(\mathbf{k})$ is spherically symmetric. Thus we can write

$$\rho(\mathbf{r}) = \frac{4\pi}{3\Omega} \int_{\text{cell}} \rho(\mathbf{r}) \, r^2 \, d^3r.$$  

(2.64)

Substituting Eq. (2.65) into Eq. (2.64) and evaluating the integral one obtains

$$\Lambda \rho(\mathbf{r}) = \sum_{K_S} \Lambda \rho(|\mathbf{K}_S|) e^{i\mathbf{K}_S \cdot \mathbf{r}}$$

(2.65)
where \( r_0 \) is the radius of the Wigner-Sitz sphere.

The exchange potential presents more difficulty because of the cube root dependence on the charge density. It was evaluated in the following way: The change in the Fourier coefficients of charge density was averaged over directions of \( K_s \) and the resulting Fourier series was summed to determine the change in charge density in an atomic cell for each spin. This was added to the starting charge density, the cube root was extracted, and a corrected exchange potential was formed. The corresponding Fourier coefficients are obtained by a numerical 96 point Gaussian integration. The procedure just described has the disadvantage that the convergence in \( \Delta \rho (K_s) \) is slower than that in \( \Delta V_c (K_s) \) by an extra factor of \( K_s^2 \) and more terms in \( \Delta V_c (K_s) \) have to be considered than necessary. An alternative procedure is to construct the iterated charge density directly from Eq. (2.61) and (2.28). This modification has been included in the self-consistency program listed in Appendix C.
The changes in the Coulomb and exchange potential were added to the Hamiltonian matrix in the following way

\[
H_{ij}(\vec{k}) = H_{ij}^O(\vec{k}) + \sum_{\vec{k}_s} (\Delta V_c(\vec{k}_s) + \alpha \Delta V_x(\vec{k}_s)) S_{ij}(\vec{k},\vec{k}_s).
\]

(2.67)

The \( H_{ij}(\vec{k}) \) was the iterated Hamiltonian while \( H_{ij}^O(\vec{k}) \) was the original Hamiltonian matrices defined in Eq. (2.30). The new Hamiltonian was again diagonalized to obtain a new set of eigenvalues and eigenfunctions. This procedure was repeated until the desired degree of convergency has been achieved. At first, our calculation employed a value of the exchange parameter \( \alpha \) close to unity (\( \alpha = 0.972 \)), which had been found to give the most satisfactory results. The charge density was sampled at 20 points in 1/48th of the Brillouin zone. Reasonably self-consistent results were obtained after about eight iterations. The resulting energy bands appeared to be unsatisfactory, both in regard to the relation of the p and d bands, and in regard to the magneton number. Estimates were made which indicated that the exchange parameter \( \alpha \) should be decreased. It appeared that \( \alpha = 2/3 \) should be employed and the self-consistent calculations were repeated with this value. The results obtained in this case appeared to be in substantially better agreement with experiment.
Our experience with the effect of exchange on the band structure is similar to that reported by Connolly.\textsuperscript{15} We found, in agreement with Connolly, that if the full Slater exchange is used, the energy of the state $L'_2$, for both spin directions, is above the Fermi energy. Hence there would be no Fermi surface neck at $L$. The reduction of the exchange potential produced by use of the Kohn-Sham-Gaspar value of the parameter $\alpha$ raises the d levels substantially more than those of p symmetry. The $L'_2$ levels are then below the Fermi surface, while the large spin splitting of the $L'_3$ states forces $L'_3$ above the surface.

Another point of practical interest has to do with the number of iterations necessary to achieve convergence. In principle, when self-consistency has been reached, the iterated potential $V_{out}^{\hat{k}_s}$ should be equal to the input potential $V_{in}^{\hat{k}_s}$ based on which $V_{out}^{\hat{k}_s}$ are evaluated. Therefore, one should be free to modify the input potential at the beginning of each iteration by using

$$V_{in}^{\hat{k}_s} = \beta V_{out}^{\hat{k}_s} + (1-\beta) V_{in}^{\hat{k}_s} \quad (2.68)$$

where the unprimed $V^{\hat{k}_s}$ are the iterated and input potentials for the last iteration. The weighting factor $\beta$ was allowed to vary between 0 and 1. We observed that the change in the Fourier coefficients of the Coulomb potential $\Delta V_{c}^{\hat{k}_s}$ oscillated rapidly about their final
convergent values in the first few iterations. This can be avoided if we choose a value of $\beta$ which will bring $\Delta V_c(\mathbf{k}_0)$ closer to their convergent values. A value of $\beta$ close to 0.3 seemed to work very well for the first few iterations for transition metals. It should be increased when the oscillations settle down, especially the change in $V_c(\mathbf{k})$ becomes monotonic. The changes in the relative position of energy levels $L_{2}', L_{3}$ and the Fermi energy produced an additional problem. The change in the Fourier coefficients apparently became divergent after a rough degree of convergence seemed to have been achieved. This was caused by oscillations in the position of $L_{2}'$ with respect to the Fermi energy and could only be solved by introducing a very small value of $\beta$. The criterion employed to define an adequate degree of self-consistency was that the Fourier coefficients of Coulomb potential should be stable to 0.002 Ry. For the case $\alpha = 2/3$, eight iterations were made using 20 points in 1/48th of the Brillouin zone, followed by three iterations using 89 points. It was sufficient to consider only Fourier coefficients of potential for the 50 shortest reciprocal-lattice vectors in the iterative procedure to achieve self-consistency. The convergence of the exchange potential is somewhat more rapid than that for the Coulomb potential.
Numerical values are presented for some Fourier coefficients in Table I. The calculated band structure is shown in Figs. II and III for electrons of majority ($\uparrow$) and minority spins ($\downarrow$) along some symmetry directions. The bands have the expected shape, showing hybridization between the relatively narrow d band complex and a broad s-p band. Certain characteristic energy differences are listed in Table II. There is a substantial degree of agreement between our values for some of these separations and the corresponding results obtained by Connolly. These energy differences are also in fair agreement with the results of Wakoh, however, this author uses the full Slater exchange ($\alpha = 1$).

Exchange splittings of certain states are given in Table III. Results from the non-self-consistent calculation ($\alpha = 0.972$), together with other self-consistent calculations, are shown for comparison. It is seen that the splitting of states of predominately d symmetry has decreased slightly but not by as much as would have been expected in view of the decrease in $\alpha$. There is significant variation in the amount of splitting from band to band. A striking result is that the splitting of states of predominately s-p symmetry is nearly zero. These results can be qualitatively explained in terms of the redistribution of spin density which will be discussed in Section A of Chapter III. The spin polarization
becomes negative (minority spin predominates) in the outer portions of the atomic cell. Highly extended states (s-p) experience cancellation of positive and negative exchange potentials. The more extended d states near the bottom of the band are also located on the average in a region of weaker exchange potential.

The self-consistent energy bands and wave functions were used to calculate the spin density, X-ray form factor and Compton profile. In the next section we discuss the inclusion of the spin orbit interaction to the self-consistent potential.

D. Spin Orbit Coupling

The calculation previously described was extended by the inclusion of spin orbit coupling. Other relativistic effects were neglected. Introduction of spin orbit coupling into a band calculation for a ferromagnet causes substantial complications. First, since spin orbit coupling connects states of $\uparrow$ and $\downarrow$ spin, the size of the Hamiltonian matrix is increased (in our case 76x76), and the elements become complex. This causes a considerable increase in computing time. Second, the symmetry group is reduced. The appropriate group theory has been presented by Falicov and Ruvalds and Cracknell. In addition the band structure depends on the direction of spin alignment. Separate band structures must be computed for each
direction spin alignment investigated. However, because of limitations of computer time, we have restricted our calculations to a single direction of spin alignment: the [001] axis.

Falicov and Ruvalds considered for inclusion in the space group: (1) the ordinary lattice translation, (2) rotation about the direction of spin alignment, \( \hat{\mathbf{n}} \), (3) the product of these rotations with the inversion, and (4) combinations of these rotation and rotation-inversion with translation. Wigner pointed out that there may be an additional symmetry to be considered. Although time reversal, by itself, is not a symmetry operation, the product of time reversal and either a two-fold rotation about an axis perpendicular to the field direction \( \hat{\mathbf{n}} \) or a reflection in a plane containing the \( \hat{\mathbf{n}} \) axis is a candidate for a symmetry operation of the crystal. A detailed discussion of the additional symmetry operations has been presented by Cracknell.

The computation of the matrix elements of the spin orbit interaction was performed as follows. The additional term in the Hamiltonian has the form

\[
\hat{\mathbf{V}}_{\text{s.o.}} = \frac{\hbar}{2m^*c^2} \mathbf{V}_c \times \mathbf{p}
\]  

(2.69)

The potential \( \mathbf{V}_c \) used in (2.69) was that obtained from the self-consistent band calculation, expressed as a Fourier
series

\[ V_c = \sum_K^{iK_s \cdot \mathbf{r}} V(K_s) e^{iK_s \cdot \mathbf{r}} \]  \hspace{1cm} (2.70)

Use of Gaussian orbitals is advantageous, as all matrix elements of the $H_{s.o.}$ can be reduced to sums of simple analytic functions of the reciprocal lattice vectors. We found in several tests that the only non-negligible matrix elements of $H_{s.o.}$ are those in the p-p and d-d blocks, with orbitals centered on the same atomic site ("central cell"). The central cell matrix elements of $H_{s.o.}$ have the following form

\[
H_{s.o.} = \begin{pmatrix}
  \uparrow & \downarrow \\
  \uparrow & v_1 & v_2 \\
  \downarrow & -v_2^{*} & v_1^{*}
\end{pmatrix}
\]  \hspace{1cm} (2.71)

in which the spin states considered are indicated by arrows. The forms of the sub-matrices $v_1$ and $v_2$ are as follows for the p-p block:

\[
\begin{pmatrix}
x_{\uparrow} & y_{\uparrow} & z_{\uparrow}
\end{pmatrix}
\begin{pmatrix}
0 & i\Lambda & 0 \\
0 & -i\Lambda & 0 \\
0 & 0 & 0
\end{pmatrix}
\]  \hspace{1cm} (2.72)
The symmetries of the basis states are indicated above and to the left of the matrix.

\[
\begin{pmatrix}
x^+ & y^+ & z^+ \\
x^+ & 0 & 0 & -A \\
p \mid v_2 \mid p^+ & = & y^+ & 0 & 0 & iA \\
z^+ & A & -iA & 0
\end{pmatrix}
\] (2.73)

In these equations,

\[A = \left(\frac{3}{4\pi}\right)N \int \frac{V(K)K^2}{F(K)}\] (2.74)

in which

\[F(K) = \frac{\hbar^2}{24mc^2} \pi^{3/2} \gamma^{5/2} \exp\left(\frac{-\gamma K^2}{4}\right)\] (2.75)

and

\[\gamma = \frac{1}{\alpha_1 + \alpha_2}\] (2.76)

The sums include all reciprocal lattice vectors; \(\alpha_1\) and \(\alpha_2\) are the exponents of the Gaussian orbitals, and \(N\) is the product of the appropriate normalization constants. The corresponding formulas for the d-d block are\textsuperscript{61}
\[
\begin{array}{cccccc}
\text{xy}^\dagger & \text{yz}^\dagger & \text{zx}^\dagger & \text{ }^2-\text{y}^2 & \text{3z}^2-\text{r}^2 \\
\text{xy}^\dagger & 0 & 0 & 0 & \text{iB} & 0 \\
\text{yz}^\dagger & 0 & 0 & \text{iC} & 0 & 0 \\
\text{zx}^\dagger & 0 & -\text{iC} & 0 & 0 & 0 \\
\text{ }^2-\text{y}^2 & -\text{iB} & 0 & 0 & 0 & 0 \\
\text{3z}^2-\text{r}^2 & 0 & 0 & 0 & 0 & 0 \\
\end{array}
\]
\quad (2.77)

\[
\begin{array}{cccccc}
\text{xy}^\dagger & \text{yz}^\dagger & \text{zx}^\dagger & \text{ }^2-\text{y}^2 & \text{3z}^2-\text{r}^2 \\
\text{xy}^\dagger & 0 & \text{C} & -\text{iC} & 0 & 0 \\
\text{yz}^\dagger & -\text{C} & 0 & 0 & -\frac{\text{iB}}{2} & -\frac{\text{i}\sqrt{3}}{2} \text{B} \\
\text{zx}^\dagger & \text{iC} & 0 & 0 & -\frac{\text{B}}{2} & \frac{\sqrt{3}}{2} \text{B} \\
\text{ }^2-\text{y}^2 & 0 & \frac{\text{iB}}{2} & \frac{\text{B}}{2} & 0 & 0 \\
\text{3z}^2-\text{r}^2 & 0 & \frac{\text{i}\sqrt{3}}{2} \text{B} & -\frac{\sqrt{3}}{2} \text{B} & 0 & 0 \\
\end{array}
\]
\quad (2.78)

where

\[
\begin{align*}
\text{r} & = \frac{15}{44} \frac{\text{N_y}}{\text{K}} \text{V}(\text{K}) \text{F}(\text{K}) [\alpha_2 \gamma^2 (K_x^4 + K_y^4 + K_z^4) \\
& + (2;1;1) \gamma^2 (K_x^2 K_y^2 + K_y^2 K_z^2 + K_z^2 K_x^2) - 4 K^2)]
\end{align*}
\quad (2.79)\]
\[ C = \frac{15}{4\pi} \frac{N_Y}{4} \sum_K V(K) F(K) \left[ \gamma (K_x^2 K_y^2 + K_x^2 K_z^2 + K_y^2 K_z^2) - 2K^2 \right] \]

(2.80)

All of the basis functions are assumed to be normalized with respect to the angular integrations so that \( N \) depends on the orbital exponents only. Spherical symmetry of the potential has not been assumed in writing these formulas. There are in this case, two independent constants involved in the d-d spin orbit Hamiltonian. In fact, spherical symmetry is a good approximation, since it is the potential close to a nucleus which is important. For a spherically symmetric potential, we have simply

\[ B = 2C = \xi, \quad (2.81) \]

where \( \xi \) is the usual spin orbit coupling parameter if atomic wave functions are employed in the usual form, \( H_{s.o.} = \xi L \cdot S \).

In our calculation, the spin orbit parameters, A, B, C, depend on the indices of the pair of orbital functions used in calculating the matrix elements. In order to compare calculations of properties of nickel which are dependent on spin orbit coupling, it is useful to compute an equivalent atomic spin orbit coupling parameter. This calculation was performed with the wavefunctions of
Wachters\textsuperscript{53} and our self-consistent potential. We found $\xi = 0.0067 \text{ Ry.}$ This result is somewhat larger than the atomic value $\xi = 0.0055 \text{ Ry.}\textsuperscript{62}$ The difference between $B$ and $2C$ was found to be zero within the accuracy of our calculation.

The Hamiltonian including exchange and spin orbit coupling was diagonalized at 1357 points in $1/16$'th of the Brillouin zone. The calculated band structure is shown along certain symmetry lines in Fig. IV. Some calculated energy levels at symmetry points are listed in Table IV. Since the actual symmetry group for this problem does not permit a particularly informative classification of states, we have labelled states at symmetry points in Fig. IV in terms of the predominant component; that is, neglecting the mixing of states of majority and minority spin components. This labelling is possible since spin orbit coupling is small compared to the exchange splitting.

It will be noticed that the band structure shown in Fig. IV is quite similar to that formed by superposing the majority and minority spin bands shown in Fig. II and III. However, spin orbit coupling removes many of the accidental degeneracies present in such a picture. The interplay of spin orbit and exchange effects can be illustrated by considering the points $X$. In the present case, there are two inequivalent points of this type which are not connected by an operation of the symmetry group: these
are denoted $X(001)$ and $X(100)$. Since the exchange splitting is large compared to spin orbit coupling, we can qualitatively consider the latter as a perturbation. Specifically, let us consider the states $X_{5\uparrow}$ near the top of the d band. For $X(100)$, the basis functions are of the symmetry $xy\downarrow$, $xz\downarrow$. Spin orbit coupling does not connect these states, instead there is coupling between these and other majority and minority spin states. Since these states are separated from $X_{5\uparrow}$, the splitting of $X_{5\uparrow}$ is small (0.0012 Ry). On the other hand, for $X(001)$, the basis function are $zy$, $zx$. There is a non-zero spin orbit matrix element between these states, leading to a considerably larger splitting (0.0078 Ry).

In the following chapter, results are presented for the charge density, the spin density, the Compton Profile, the density of states, the Fermi surface, and the optical conductivity tensor. A detailed comparison of theory and experiment is attempted.
CHAPTER III
APPLICATIONS AND RESULTS

In this chapter the energy and wavefunctions obtained in our calculation are compared with experiment. We present in Section A the spin and charge density. Section B contains a discussion of the method employed to calculate the momentum distribution of electrons in solids. The procedure used to calculate the density of states is described in Section C. Our results for Fermi surface properties are presented in Section D and are compared with experiment. Finally, the calculation of the optical conductivity is summarized in Section E.

Section A. Spin and Charge Density

The Kohn-Sham-Gaspar exchange prescription is based on a variational calculation of the total energy, regarded as a functional of the charge density. It is therefore particularly interesting to examine the results of our calculation with respect to the charge density. Some calculated charge densities along three main crystallographic directions are listed in Table V. Contribution from the band electrons has been separated in the table. Figure V shows the band electron charge densities $\rho_b(\mathbf{r})$ along [100], [110], and [111] directions. The spherical average Hartree-Fock atomic charge densities based on
are also included for comparison. The ground state atomic configuration \((3d^8, 4s^2)\) was employed. There is considerable asymmetry in the charge distribution as \(n_\text{b}(\mathbf{r})\) is spread out along the [100] direction relative to the [110] and [111] directions.

The contact charge density \(n_\text{b}(0)\) in the solid differs from that in the atom as a result of two principal effects. First, the s wave functions are normalized within an atomic cell. This tends to increase \(n_\text{b}(0)\) relative to a free atom. Second, hybridization mixes d and p components into a s band. This tends to reduce \(n_\text{b}(0)\). There is some partially compensating increase due to inclusion of s character into primarily d-like bands. The final result for \(n_\text{b}(0)\) is not greatly different from the free atom value.

The theoretical results for the Fourier coefficients of the charge density can be compared with experimental observations of the X-ray atomic scattering factor by Diana, Mazzone, and De Marco. The results are presented in Table VI. The small differences between the theoretical values for \(\mathbf{K}_{[333]}\) and \(\mathbf{K}_{[511]}\) and between \(\mathbf{K}_{[600]}\) and \(\mathbf{K}_{[442]}\) indicate slight departures of the charge distribution from spherical symmetry. Although there are deviations between theory and experiment which are outside the quoted experimental error, we feel that the agreement is fairly good. In the case of the [111], [200] vectors, our
results are significantly closer to experiment than are values calculated from free atom Hartree-Fock charge densities for either $d^8s^2$ or $d^{10}$ configurations and reported by Diana et al.

The distribution of spin density in nickel has been investigated by Mook through neutron diffraction. This experiment determines a magnetic form factor, $f(\mathbf{K})$, which is the ratio of the magnetic scattering amplitude for a scattering vector $\mathbf{K}$, to that for $\mathbf{K}=0$. This function has been computed by Hodges, Ehrenreich, and Lang using their combined tight-binding and pseudopotential interpolation method. It is customary to express $f(\mathbf{K})$ as the sum of three terms

$$f(\mathbf{K}) = \frac{2}{g} f_{\text{spin}}(\mathbf{K}) + \frac{(g-2)}{q} f_{\text{orb}}(\mathbf{K}) + f_{\text{core}}(\mathbf{K})$$

(3.1)

in which $g$ is the spectroscopic splitting factor and has been determined to be 2.18 for Ni. The quantity $f_{\text{spin}}$ is the form factor for the unpaired (mainly d) electrons, and is normalized so that $f_{\text{spin}}(0) = 1$:

$$f_{\text{spin}}(\mathbf{K}) = (N\nu)^{-1} \left\{ e^{i\mathbf{K} \cdot \hat{r}} \left[ \rho^+(\mathbf{r}) - \rho^-(\mathbf{r}) \right] \right\} d^3r$$

(3.2)
in which \( v \) is the magneton number. Although the core has a net spin of zero, exchange effects produce a slight difference in the radial distributions of \( \uparrow \) and \( \downarrow \) spin core electrons, and so, lead to a small contribution \( f_{\text{core}} \). Finally, there is a contribution, \( f_{\text{orb}} \) from the possible unquenched orbital angular momentum of the d electrons. This term has been studied by Blume. However, the assumptions of this calculation are not in accord with the band picture described here.

We have calculated the spin and core contributions to \( f(\hat{K}) \), using the wavefunctions obtained from our band calculation. The formulas are obtained immediately from Eq. (2.62) and the results are tabulated in Table VII. The magnetic form factors are shown in Fig. VI where they are compared with the experimental values of Mook. A satisfactory, although not perfect degree of agreement is obtained. It will be noted that there can be considerable departures from spherical symmetry: \( f(\hat{K}) \) is not simply a function of \( |\hat{K}| \), in agreement with experiment.

It is also of interest to examine the position dependence of the spin density \( f_\uparrow(\hat{r}) - f_\downarrow(\hat{r}) \). Results are shown in Fig. VII and Table VIII. Contribution from the core and band electrons are separated in the table. In contrary to the results of the charge distribution, the magnetic moment densities in [111] and [110] directions
are larger than that in [100] direction. This result is in agreement with Mook's analysis. The contribution to the contact charge density from electrons of minority spin is slightly larger than that from electrons of majority spin.

It will be noted that the spin density is negative at large values of $\mathbf{r}$, indicating that there is a net negative spin polarization in the outer portion of the atomic cell. This result is also in agreement with the measurement of positron annihilation.\(^6\)

B. Momentum Distribution of Electrons

Recently, there has been a renewed interest in the Compton scattering experiments in solids. Unlike X-ray scattering factors, which are insensitive to the outer electron charge density, the Compton measurements are sensitive to the momentum distribution of outer electrons. Thus the Compton scattering experiments can provide a critical test for the wavefunctions from energy band calculation.

Platzman and Tzoar, by considering time dependent scattering theory, justified the use of the impulse approximation in the theory of Compton line shape.\(^6\) The result can be summarized as follows: The impulse approximation is valid if (1) the wavelength of the incident photon is so short that it interacts with only
a single electron and ejects it instantaneously from the Fermi sea, (2) the energy transferred to the electron is large enough that the collision time is much shorter than the time required for any rearrangement of the remaining electrons. The net effect is that the photon exchanges energy and momentum with a single electron in a constant potential field. The differential scattering cross section of photons from a system of electrons in solid can be shown to be

\[
\frac{d\sigma}{d\omega d\Omega} = \left(\frac{e^2}{mc^2}\right)^2 \left(\hat{r}_1 \cdot \hat{r}_2\right)^2 \left(\frac{\omega_2}{\omega_1}\right) \frac{m}{\hbar} \frac{1}{|\hat{k}|} J^k_\gamma(q) . \tag{3.3}
\]

The Compton profile is given by

\[
J^k_\gamma(q) = \frac{\omega}{2\pi} \int d^3\mathbf{p} \nu(\mathbf{p}) \delta(q - \mathbf{p} \cdot \hat{k}) \tag{3.4}
\]

with

\[
\hat{k} = \frac{\mathbf{k}}{|\mathbf{k}|} \tag{3.5}
\]

and

\[
q = \frac{m\omega}{|k|} - \frac{|\mathbf{k}|^2}{2} . \tag{3.6}
\]

Here \(\hat{r}_1, \hat{r}_2, \hat{k}_1, \hat{k}_2\), and \(\omega_1, \omega_2\) are the polarization, momentum and frequency of the incident and the scattered
photons respectively, $\mathbf{k} = \mathbf{k}_1 - \mathbf{k}_2$ and $\omega = \omega_1 - \omega_2$ are the momentum and energy transferred to the electrons, and $\mathcal{V}$ is the volume of a primitive cell. The delta function appearing in Eq. (3.4) is deduced from the energy conservation

$$\omega = \frac{|\mathbf{k}|^2}{2m} - \frac{\mathbf{k} \cdot \mathbf{p}}{m}.$$  

(3.7)

The scattered photon is shifted in energy both by the momentum transfer $k'^2/2m$ and the doppler shift component $(\mathbf{k} \cdot \mathbf{p}/m)$. The momentum distribution function which also appears in Eq. (3.4) gives the probability of finding the initial electron with a given momentum $\mathbf{p}$.

$$\rho (\mathbf{p}) = \sum_{\mathbf{g}} |\psi_n (\mathbf{g}, \mathbf{p})|^2.$$  

(3.8)

The summation in Eq. (3.8) includes occupied states specified by band index $n$ and wavevector $\mathbf{g}$ and $\psi_n (\mathbf{g}, \mathbf{p})$ is the Fourier transform of the Bloch wavefunction $\psi_n (\mathbf{g}, \mathbf{r})$

$$\psi_n (\mathbf{g}, \mathbf{r}) = \frac{1}{\sqrt{N}} \int e^{-i \mathbf{p} \cdot \mathbf{r}} \psi_n (\mathbf{g}, \mathbf{r}) \, d^3 \mathbf{r}$$

$$= \sum_{\mathbf{k}_S} a_{n\mathbf{k}_S} (\mathbf{g}) \delta (\mathbf{p} - \mathbf{k}_S - \mathbf{K}_S) \chi_i (\mathbf{p})$$  

(3.9)

where the second summation runs over all reciprocal lattice vectors $\mathbf{k}_S$, $a_{n\mathbf{k}_S} (\mathbf{g})$ is the expansion coefficients of the crystal wavefunctions, and $\chi_i (\mathbf{p})$ is the Fourier
transform of the atomic wavefunctions \( u_i(r) \)

\[
\chi_i(\vec{p}) = \frac{1}{\sqrt{n_i}} \int e^{-i\vec{p} \cdot \vec{r}} u_i(\vec{r}) \, d^3r.
\]  

(3.10)

The expressions for \( \chi_i(\vec{p}) \) are given in Appendix A. The integral in Eq. (3.4) implies that the Compton profile measures the number of electrons having a fixed value of momentum in the direction of the photon's scattering vector \( \hat{k} \).

Neglecting spin-orbit interaction, the expansion coefficients \( a_{ni}(\vec{g}) \) have been tabulated for 89 independent points in \( 1/48 \)th of the Brillouin zone. The summation over all \( \vec{g} \) in the Brillouin zone may be expressed in terms of a sum over \( \vec{g} \) in the primitive \( 1/48 \)th of the zone and a sum over group operations which generate the star of \( \vec{g} \). The symmetry properties of the Bloch function can then be used to transform the variables of integration. The final form of the expression for the Compton profile is

\[
J^\hat{k}(\vec{q}) = \frac{\hbar}{(2\pi)^3} \sum_{\text{occ}} \int_{\vec{g} \in \{1\}}^{1 \text{\ 48 \th}} d^3g \frac{1}{48} \chi_i(\vec{g}+\vec{k}_s) \left| a_{ni}(\vec{g}) \right|^2
\]

\[
\times \hat{\Sigma}_i \left[ \vec{q} - (\vec{g}+\vec{k}_s) \cdot \vec{\beta} \hat{k} \right].
\]  

(3.11)

The sum over \( \beta \) includes all operators in the cubic point group.
If a GTO involves the factor $e^{-ar^2}$ its Fourier transform will be proportional to $e^{-p^2/4a}$. These factors govern the convergence of the sum over reciprocal lattice vectors in Eq. (3.11). For band states, the effective $a$'s are not large and good convergence is obtained. However, convergence is much slower for core functions where large $a$'s are encountered. A check on convergence can be obtained from the normalization condition on $J_K(q)$:

$$\int_{-\infty}^{\infty} J_K^c(q) dq = n_e$$

(3.12)

in which $n_e$ is the number of electrons per atom. In our calculation, the sums over $K_s$ were carried out over approximately 3000 permuted reciprocal lattice vectors. No contribution was included from the 1s wavefunctions (the impulse approximation is probably not valid for 1s electrons in X-ray Compton scattering measurements). The convergence of the reciprocal lattice sum for the band (3d and 4s) electrons is quite good; however, it is not complete for the core electrons. There remain small contributions, mostly from the 2s and 2p electrons, that have been neglected. Consequently, the theoretical curves are probably slightly too low. This effect will be important mainly for larger values of $q$ than are studied here. The contribution from the 1s electrons was determined using atomic wavefunctions. This was included in
our calculation in order to compare with the experimental results using high energy $\gamma$ rays.

The Compton profile in [100], [110], and [111] directions are shown in Fig. VIII. The contribution from core electrons (2s, 2p, 3s, 3p) has been separated from the total in the figures. The difference in Compton profiles along different directions is illustrated in Fig. IX. The experimental measurements of Eisbergen and Reed are also included for comparison. Considerable structure is evident in the curves. Much of this structure can be attributed to Fermi surface effects. The momentum density $\rho(p)$ suffers some discontinuity whenever $\hat{p}$ touches a piece of Fermi surface. For a fixed direction of momentum transfer $\hat{k}$, the Compton profile $J^K(q)$ measures the amount of the momentum density, contained in a plane perpendicular to $\hat{k}$, sweeping through the momentum space. The profile will have a cusplike behavior when the plane perpendicular to $\hat{k}$ happens to be tangent to a piece of flat Fermi surface. A thorough measurement on the Compton line shape can, therefore, provide information on the shape of the Fermi surface. Similar structures corresponding to Fermi surfaces in the higher order of the Brillouin zone should exist for larger values of $q$. The sharpness of the breaks in $J^K(q)$ indicates the amount of discontinuity presented in $\rho(p)$. The periodicities in the anisotropy of the Compton profile along different directions reflect
the position of the reciprocal lattice vectors and hence the size and structure of the primitive cell. Of course, many body effects would be expected to reduce the visibility of these structures through the introduction of additional high momentum components into the band wavefunctions.

The Compton profile along the [1,0,0] direction is relatively smooth since most of the Fermi surfaces parallel to this direction are moderately spherical. (See Figs. XIV and XV). The structures presented in $J_{[1,1,0]}(q)$ and $J_{[1,0,0]}(q)$ can be understood based on the Fermi surface effects along the [1,1,0] direction. The fine structure near the origin reflects the anisotropy in the dimensions of the X hole pockets. The structures near 0.45 and 0.58 a.u. correspond to the two square pieces of the Fermi surface centered at $\Gamma(0,0,0)$. Similarly, structures near 0.76, 0.89, 1.79, and 1.92 a.u. correspond to those centered at $2\pi/a(1,1,1)$ and $2\pi/a(2,0,0)$. Fine structures near the $\Gamma$ points displaced by a reciprocal lattice vector to locations of magnitude 1.34, and 2.68 a.u. when projected onto the [1,1,0] direction, can be attributed to the effects of X hole pockets. The rapid raise near the origin in $J_{[1,1,1]}(q) - J_{[1,0,0]}(q)$ reflects the difference in the cross sectional area of the $\Gamma$ centered electron Fermi surfaces. The contributions from the $L_{2}^{\dagger}$ necks are resolved in this picture into two small bumps near 0.27
a.u.. Fine structures near 0.82 and 1.36 a.u. correspond to \( L_2^\dagger \) centered at \( 2\pi/a(2,0,0) \). The minima near 0.55 and 1.64 a.u. can be attributed to the cross sections of the X hole pockets in the plane perpendicular to the \([1,1,1]\) direction. Finally, the structures in \( J_{[1,1,0]}(q) \) and \( -J_{[1,1,1]}(q) \) can be interpreted as the combination of the Fermi surface effects described above.

The spherical average Compton profile was obtained using a sixth order Kubic harmonics expansion. The spherical average \( J_{av}(q) \) was approximated as the zeroth order term in the expansion. The results are compared with x-ray Compton scattering measurements \(^{71,72}\) in Fig. X. The contributions from occupied band states are also included for detailed comparison. The contribution from the atomic core states that we used to subtract from the experimental measurements has been tabulated in Ref. 71. The agreement is reasonably good except for large values of \( q \) in the total \( J_{av}(q) \). This discrepancy may be attributed to many body effects. Numerical values for the Compton profile and the contribution from band electrons can be found in Tables IX and X respectively.
C. The Density of States

Gilat has reviewed different methods of calculating the density of states. We employ here the Gilat-Raubenheimer method in combination with an interpolation scheme. The method is similar to that used by Cooke and Wood, except that our interpolation procedure is based on second order \( \mathbf{k} \cdot \mathbf{p} \) perturbation theory. The band calculation with spin orbit coupling included 1357 points in 1/16'th of the Brillouin zone. Energies, wave functions, and momentum matrix elements were obtained at these points. A finer mesh was constructed by dividing the original step size by three -- this represents 26 additional points around each previous general point. The \( \mathbf{k} \cdot \mathbf{p} \) calculation was performed as follows. If a given band at the "original" point \( (\mathbf{k}_0) \) was separated by 0.005 Ry or more from all other bands ordinary perturbation theory was employed to determine the energy at the additional points \( (k) \). Thus

\[
E_n(k) = E_n(k_0) + \frac{\hbar}{m} (k-k_0) \cdot \pi_{nn} + \frac{\hbar^2}{2m} (k^2-k_0^2)
+ \frac{\hbar^2}{m^2} \sum_{j(j\neq n)} \frac{[(k-k_0) \cdot \pi_{nj}][(k-k_0) \cdot \pi_{jn}]}{E_n(k_0)-E_j(k_0)}
\]

(3.13)
The matrix element is

\[
\hat{\eta}_{nj} = \frac{(2\pi)^3}{h^3} \int \left[ W_n^* (k_O, r) \left( \frac{\hbar}{4mc^2} \hat{\mathbf{a}} \cdot \nabla V(r) \right) W_j (k_O, r) \right] d^3 r
\]

(3.14)

in which \( h^3 \) is the volume of the cell and \( W \) is the cell periodic part of the Bloch function.

\[
W_n (k, r) = e^{-i\mathbf{k} \cdot \mathbf{r}} \psi_n (k, r).
\]

(3.15)

Numerical tests showed that the spin orbit contribution to the matrix element (the term in (3.14) proportional to \( \hat{\mathbf{a}} \cdot \nabla V \)) was negligible; hence in practice \( \hat{\eta}_{nj} \) was always replaced by \( \hat{\eta}_{nj}' \). Only 12 bands were included in the sum in (3.13). Thus, the second order term is not computed exactly, but since the other energy denominators are much larger, the accuracy should be sufficient. When two or more bands at \( k_O \) were separated by less than 0.005 Ry, an effective Hamiltonian was diagonalized. The elements of this Hamiltonian are

\[
H_{nm} (k) = \left[ E_n (k_O) + \frac{\hbar^2}{2m} (k-k_O)^2 \right] \delta_{nm} + \frac{\hbar}{m} (k-k_O) \cdot \hat{\eta}_{jn}
\]

(3.16)
in which $E_A$ is the average energy of the nearly degenerate levels at $k_0$. The prime on the sum indicates that the nearly degenerate levels are excluded. As before, only twelve bands were included in the sum in Eq. (3.16), so that second order term is not exact.

The linear analytic integration scheme was then applied to each minicell constructed around each mesh point. Projection operators were used to separate the contributions from majority and minority spins to the density of states. Our results for the majority and minority spin state densities and for the total are shown in Figs. XI-XIII. The total density of states at the Fermi energy was found to be 23.56 electrons/atom-Ry. The electronic specific heat coefficient $\gamma = \frac{\pi^2}{3} \frac{N(E_F)k^2}{N} \frac{E^2}{k}$, where $k$ is the Boltzman's constant, was found to be 4.08 mJ/ (mol °K2). Measurements of the low temperature specific heat yield a value of 7.028 mJ/(mol °K2). Part of the discrepancy may be attributed to neglect of the electron-phonon interaction. The magneton number was found to be 0.62, somewhat higher than the experimental value of 0.56. Our calculation predicts that a minority spin hole pocket associated with the $X_2^+$ level should exist. This has not been observed experimentally, although it has also been predicted by other self-consistent calculations. This hole pocket is probably responsible for the disagreement between theoretical and experimental values of the
magnetron number.

D. The Fermi Surface

The Fermi surface of nickel has been carefully studied through measurements of the de Haas-van Alphen effect and cyclotron resonance. These observations are of great importance in that they confirm the general picture of itinerant electron ferromagnetism in nickel, in which the electrons responsible for magnetic order are not localized, but instead have wave functions extending throughout the crystal and contribute to the formation of a Fermi surface.

The major features of the Fermi surface of nickel can be understood on the basis of a calculation in which spin orbit coupling is neglected, but this interaction must be included in a detailed comparison of theory and experiment. As was noted above, the spin orbit splitting of the states \( X_{5+} \) (001) and \( X_{5+} \) (100) is quite different. This leads to a significant difference in the sizes of the hole pockets around these points and to large anisotropy of de Haas-van Alphen frequencies. A rapid variation of the de Haas-van Alphen amplitude when the applied magnetic field is tilted a few degrees from the [110] direction in a (110) plane has been interpreted as resulting from magnetic breakdown across a small gap resulting from the removal of an accidental degeneracy between spin
orbit split bands.\textsuperscript{20}

In our calculation, spins are quantized along the [001] axis. We are therefore limited in principle to an investigation of the Fermi surface in the \( k_z \) constant planes. However, the dependence of the band structure on the field direction is probably not large except for the small hole pockets at \( X \), and we will discuss cross sections in a (1\( \bar{1} \)0) plane as well. Our Fermi surface cross sections shown in Figs. XIV and XV, where they are compared with recent results of Stark\textsuperscript{81} for the large portions of the surface and of Tsui\textsuperscript{80} concerning the hole pocket at \( X \).

Stark has derived Fermi surface radii from his measurements using the Cubic Harmonic expansion method of Mueller and Priestly.\textsuperscript{83} His inversion program included seven Cubic Harmonics. We have plotted the Fermi surface radii obtained in this manner on the figures. An empirical formula given by Tsui has been used to outline an experimentally determined cross section for the small hole pocket at \( X \).

Some numerical results for dimensions of the \( X_5 \) hole pocket are given in Table XI and extremal areas are listed in Table XII. Comparisons are made with experiment\textsuperscript{79,80,81} and with the calculations of Zornberg.\textsuperscript{22}

There is a substantial degree of agreement between the theoretical and experimental results. It is apparent that the band calculation is able to describe the major pieces of Fermi surface correctly. The most significant
disagreement concerns the $X_{2+}$ hole pocket, which is not observed experimentally, but is predicted by our calculations. Since this pocket is predicted by other band calculations using a local exchange potential, it is possible that this prediction indicates a basic inadequacy of the local exchange approximation.

The majority-spin portion of the Fermi surface lies entirely in the upper s-p band. The surface is in contact with the Brillouin zone near the points L. A neck of roughly circular cross section is formed at each such point. We obtained a value of 0.0035 a.u. for the cross sectional area of this neck in the hexagonal face of the zone. This is smaller than the experimental measurement of 0.0072 a.u. obtained by Tsui. It is probable that the $L'_{2+}$ level is too close below the Fermi level due to insufficient variational freedom in the s-p type basis functions which are expanded in atomic orbitals. The wave function associated with the $L'_{2+}$ state has pure p-type symmetry. Only the p-p block needs to be considered to investigate this problem. The $L'_{2+}$ level calculated by expanding the basis functions in ten individual GTO for each type of p symmetry ($x, y, \text{and} z$) lies 0.008 Ry below that of atomic GTO. The Gaussian exponents used were the same as the one for atomic GTO. But the smallest exponent was not included because it gave rise to a negative eigenvalue in the overlap matrix. A rough
estimate of the new cross sectional area was made after raising the Fermi energy with respect to the \( \Delta_{1\downarrow} \) level by 0.008 Ry. The result is 0.0068 a.u., in good agreement with the measurements of Tsui.

Goy and Grimes\(^8^2\) have observed cyclotron resonance associated with the majority spin Fermi surface neck at \( L \), the hole pocket \( X_5 \) and, according to our interpretation, the two large pieces of Fermi surface around \( \Gamma \). The wave functions associated with the smaller piece have predominantly \( e_g \) symmetry near the \( \Gamma-X \) line, but mixed components of \( s-p^+ \) and \( t_{2g^+} \) near \( \Gamma-K \). The states associated with the larger, nearly square section, are of predominantly majority spin but have the same spatial symmetry as those on the smaller square, except near the \( [100] \) axis where there is a strong, spin orbit induced mixing with minority spin \( d \) band states.

The experimentally observed cyclotron effective mass has been compared with the effective mass \( m_C^* \) obtained from the band structure according to the formula

\[
\frac{m_C^*}{m} = \frac{h^2}{m} \left( \frac{dA}{dE} \right) E_F.
\]

in which \( m \) is the free electron mass, and \( A \) is the area of the cyclotron orbit. Our results and the experimental findings are presented in Table XIII. The results of the semi-empirical calculation of Zornberg\(^2^2\) are also
shown. It will be seen that the agreement is fairly good for the $X_5$ pocket, with the deviation between theory and experiment being of the amount and direction expected to allow for a reasonable enhancement through the electron-phonon and the electron-magnon interactions. However, our result for the minority spin square is larger than the experimental value, while that for the majority spin square is much smaller than that observed.

E. Optical Conductivity

The optical properties of nickel have been the subject of intensive studies for a long time. As a result of difficulties in sample preparation, accuracy of the measurements, and data analyses the agreement among different experiments has frequently been poor. Therefore, a first principles calculation of optical conductivity is desired to settle some of the controversies as well as to improve our understanding of the electronic structure.

We have calculated the interband optical conductivity of nickel. We will present results in two cases: (1) including a phenomenological constant relaxation time $\tau$, and (2) in the limit $\tau \to 0$ so that the band states are sharp. The general expression can be obtained from the Kubo formula.
\[ v_{q,\omega}(\dot{q},\omega) = -\frac{Ne^2}{im_0}\delta_{\alpha\beta} + \frac{1}{\hbar\omega} \int_{-\infty}^{\infty} dt \cdot [J_{\alpha}(\dot{q},0)] \cdot e^{-i\omega t} \]

\[ J_{\beta}(\dot{q},t) = e^{-iH_0 t} \cdot J(\dot{q}) \cdot e^{iH_0 t} \] (3.18)

where \( q, \omega, \) and \( N \) are the wave vector, frequency and the electron density respectively. \( J_{\alpha}(\dot{q},t) \) are the Cartesian components of the Fourier transform of the current operator of the system in the interaction picture.

\[ \hat{J}(\dot{q},t) = e^{-iH_0 t} \cdot J(\dot{q}) \cdot e^{iH_0 t} \] (3.19)

in which \( \hat{H}_O \) is the Hamiltonian of the system in the absence of the external field. The ensemble average \[ \langle ... \rangle \] is to be computed with the equivalent density matrix \( \rho_o = e^{-\beta H_0} \), where \( Z = \text{Tr}(e^{-\beta H_0}) \) is the usual partition function. We are concerned with energy in the optical and infrared region. The corresponding photon wavelength is large compared to the lattice constant. Consequently, the spatial variation of the electric field over the unit cell can be neglected and it is sufficient to consider the limit \( \dot{q} \to 0 \) only. Denoting \( \dot{J}(t) = \dot{J}(\dot{0},t) \), it can easily be verified that

\[ [J(0), J(\dot{0})] = \frac{1}{Z} \cdot e^{-\beta H_0} \cdot [i \cdot i \cdot i \cdot i \cdot i] \cdot e^{i\omega_i t} \]

\[ - i \cdot [i \cdot i \cdot i \cdot i \cdot i] \cdot e^{i\omega_i t} \] (3.21)
in which \(|i>, |j>\) are eigenstates of \(H_0\) with eigenvalue \(E_i, E_j\) and \(H_{ij} = E_i - E_j\). At zero temperature, further simplification is possible within the Hartree Fock approximation. In this case the wave function of the system is considered to be Slater determinant of single particle Bloch functions \(\psi_n(k, r)\). Since the current operator \(\hat{J}\) for the system is the sum of one particle operators \(\hat{J}_s\), the possible matrix elements \(\langle j| \hat{J} |i\rangle\) involve the excitation of a single particle from a state \(\psi_\phi(q, r)\) which is occupied in the ground state of the system to some unoccupied state \(\psi_n(k, r)\)

\[
\langle \hat{q}|J_s|\hat{n}_k\rangle = -\frac{e}{m}\langle \hat{q}|\hat{n}|\hat{n}_k\rangle = -\frac{e}{m}\psi_n(k)n_\hat{k}\hat{q}
\]

(3.22)

where \(n_\hat{k}\) is the matrix element defined in Eq. (3.4).

We can rewrite Eq. (3.21) in the following form:

\[
\left[J_x(0), J_y(t)\right]_0 = -\frac{e^2}{m^2} \sum_{\hat{k}} n_{\hat{k}}^{\alpha} \left(n_{\hat{k}}^{\beta} (k) n_{\hat{n}}^{\alpha} (\hat{k}) - n_{\hat{n}}^{\beta} (k) n_{\hat{k}}^{\alpha} (\hat{k}) \right) \left[\psi_{\hat{n}}^\beta (\hat{k}) \psi_{\hat{n}}^\alpha (k) e^{i\omega_{\hat{n}} (\hat{k}) t} - \psi_{\hat{n}}^\alpha (k) \psi_{\hat{n}}^\beta (\hat{k}) e^{-i\omega_{\hat{n}} (\hat{k}) t}\right]
\]

(3.23)

For convenience we employ discrete normalization.

\(\omega_{\hat{n}} (k)\) is the energy difference between band \(n\) and 1
\[
\omega_{n\nu}(\vec{k}) = \frac{1}{\hbar} (E_n(\vec{k}) - E_{\nu}(\vec{k}))
\] (3.24)

The sum over \(k, k'\) include occupied states (\(o\)) only while that over \(n, \nu\) include unoccupied states (\(u\)) only. Eq. (3.23) is inserted into Eq. (3.18). We considered the frequency \(\omega\) to have a positive imaginary part \(i/\tau\) so that the integral in Eq. (3.18) will converge at the lower limit. The result is

\[
s_{n\nu}(\omega) = \frac{-Ne^2}{im(\omega + i/\tau)} \bar{\delta}_{\alpha\beta} + \frac{ie^2}{\hbar m^2(\omega + i/\tau)} \sum_{k\nu} \sum_{k'\nu'} \frac{n^{\alpha}_{\nu}(\vec{k}) \pi^{\beta}_{\nu}(\vec{k})}{\omega + \frac{i}{\tau} - \omega_{n\nu}(\vec{k})} - \frac{\pi^{\alpha}_{\nu}(\vec{k}) \pi^{\beta}_{\nu}(\vec{k})}{\omega + \frac{i}{\tau} + \omega_{n\nu}(\vec{k})}
\] (3.25)

Further simplification is possible if one introduces the optical effective mass:

\[
\frac{N}{m^*} = \frac{1}{m^* \epsilon(\vec{k}) \epsilon_{\nu}}
\] (3.26)

where

\[
\frac{N}{m^* \epsilon(\vec{k}) \epsilon_{\nu}} = \delta_{\alpha\beta} + \frac{2}{\hbar m^*} \text{Re} \frac{(n^{\alpha}_{\nu} n^{\beta}_{\nu})}{\omega_{n\nu}}
\] (3.27)

and the sum in (3.26) includes all \(n\). The final expression for the conductivity tensor is
The ordinary optical properties of ferromagnetic nickel are determined by the diagonal components of \( \mathbf{\sigma} \) (we have \( \sigma_{xx} \neq \sigma_{yy} \neq \sigma_{zz} \), \( z \) being the direction of spin alignment). The result of setting \( \alpha = 0 \) in (3.28) is

\[
\sigma_{\alpha\alpha}(\omega) = \frac{i N e^2}{(\omega + \frac{i}{\tau}) m_{\alpha\alpha}} - \frac{2ie^2}{m^2 \gamma} \frac{\gamma}{\omega - (\omega + \frac{i}{\tau})^2}
\]

It can be directly verified that this expression satisfies the sum rule

\[
\int_0^\infty \text{Re}(\sigma_{\alpha\alpha}) d\omega = \frac{\pi N e^2}{2m}
\]

where \( m \) is the free electron mass. The first term in Eq. (3.29a) is the usual Drude formula with relaxation time \( \tau \). In the limit in which the band states are sharp \( (\gamma = 0) \), we obtain the familiar expression for the real part of the conductivity for positive frequencies.
\begin{align*}
\text{Re}[\sigma_{\alpha\beta}(\omega)] & = \frac{\pi Ne^2}{2(m^*)_{\alpha\beta}} \delta(\omega) + \frac{\pi e^2}{m^2|\omega|} \sum \sum |\pi_{\alpha\beta}^o|^2 \delta(\omega - \omega_{\nu\nu'}) \\
(3.29b)
\end{align*}

The off diagonal components of the conductivity vanish except for \( \sigma_{xy} = -\sigma_{yx} \). In this case, we have

\begin{align*}
\sigma_{xy} & = \frac{2e^2}{m^2|\omega|} \sum \sum \frac{\text{Im}(\pi_{\alpha\beta}^x \pi_{\gamma\nu}^y)}{\omega_{\nu\nu'}^2 - (\omega + \frac{1}{n^2})^2} \\
(3.31a)
\end{align*}

The sharp limit of this formula is, for positive frequencies,

\begin{align*}
\text{Im}[\sigma_{xy}(\omega)] & = \frac{\pi e^2}{m^2|\omega|} \sum \sum \frac{\text{Im}(\pi_{\alpha\beta}^x \pi_{\gamma\nu}^y)}{\omega_{\nu\nu'}^2 - (\omega - \omega_{\nu\nu'})} \\
(3.31b)
\end{align*}

If the matrix elements in these expressions are treated as constants, the conductivity is proportional to the joint density of states. We have computed this quantity by the same method described in Section C in connection with the ordinary density of states. The joint density of states shown in Fig. XVI is dominated by an enormous spike, resulting from the nearly parallel upper d bands, especially in the region X-W-L. However, the approximation in which the matrix elements are treated as
constant is a bad one since in particular the transition associated with this spike has a very weak matrix element. (The states involved in the spike are predominately of opposite spin, and the matrix element would vanish except for the mixing of opposite spin components in the wave function).

We have calculated the optical conductivity including the k dependence of all matrix elements both in the sharp limit, Eqs. (3.29b) and (3.31b) and with the inclusion of a relaxation time. The integration was performed by the method described in Section C in which the k·p method was used to calculate the energy for k corresponding to a subdivided mesh in the Brillouin zone. The momentum matrix elements at the additional mesh points were found by linear interpolation between the values calculated at the basic 1357 point grid. Numerical tests showed that the contribution of the spin orbit coupling term to the matrix element \[ n \] (Eq. (3.14)) was negligible for the determination of both the diagonal and off diagonal elements of the conductivity. We therefore replaced \[ n \] by \[ p \] throughout the calculation. This implies that the off diagonal conductivity should be regarded as being produced by the modification of the band wave functions produced by the spin-orbit interaction.

Our results for the real part of \( \sigma_{xx} \) between 0 and 1.2 eV are shown in Fig. XVII. The solid line represents
the contribution from the interband conductivity in the sharp limit \((\tau \omega)\) to which has been added an empirical Drude term,

\[
\sigma_D(\omega) = \frac{\sigma_0}{1 + \omega^2 \tau^2},
\]

in which the constants have been taken to be \(\sigma_0 = 18.6 \times 10^{15}\) sec\(^{-1}\) and \(\tau = 11.3 \times 10^{-15}\) sec, as determined by Lenham and Treherne.\(^8^5\) The dashed curve is the sum of the same empirical Drude term plus an interband contribution computed assuming essentially the same \(\tau\). We have also computed \(\text{Re}(\sigma_{zz})\), which is not the same as \(\text{Re}(\sigma_{xx})\) in the present case. However, the differences are quite small and are not significant on the scale of this graph.

The conductivity in the energy region 1.0-6.0 eV is shown in Fig. XVIII. The experimental results of several authors\(^8^6-9^1\) are also shown in these figures. Although there is a large amount of scatter in the experimental data, there is a reasonable degree of general agreement between many of the measurements, particularly in regard to the magnitude and the general trend. There is less agreement in regard to detailed structure. We believe that it is significant that our calculations are in good agreement with the general magnitude of the observed conductivity in the low energy region. In particular, the departure from the Drude term seems to be given.
satisfactorily. There is little agreement between theory and experiment in regard to specific structures at low energies except, possibly in the 0.2-0.5 eV region where structure in our calculated conductivity appears in some of the observations and is confirmed by thermoreflectance measurements.

A most important feature of our calculated results is the peak at 0.80 eV which results from transitions between the nearly parallel upper d bands near the zone face. This transition is a direct measure of the exchange splitting responsible for ferromagnetism. This peak is quite pronounced when the band states are considered to be sharp; however, it is much reduced if reasonable allowance is made for finite lifetimes of the states. We do not notice any comparable structure in the experimental data in this energy region, and we infer from this discrepancy that our calculation has probably overestimated the exchange splitting. It is not obvious from the data available to us whether or not this transition has actually been observed; however, we tentatively suggest that the broad rise beginning at 0.5 eV in the results of Lynch et al.\textsuperscript{87} may be associated with this transition. If this interpretation is correct, the d band exchange splitting is about 0.5 eV, in fair agreement with other estimates,\textsuperscript{22} and significantly smaller than our calculated value.
Some structure is present in our calculated conductivity in the 2-3 eV range, but this is much reduced when lifetime broadening is included. Failure to observe structure in this energy range suggests that lifetime effects are indeed appreciable. At higher energies, the experimental conductivity shows a large increase, beginning near 4 eV. A corresponding feature is present in our results, but it is displaced to higher energies by about 1 eV. In our calculations, this peak results from transitions between the lower s-d bands and the s-p bands above the Fermi energy. The bands involved are in the outer part of the Brillouin zone, along the X axis, and in the vicinity of the symmetry points X and L. The discrepancy in energy between theory and experiment is probably an indication of the inadequacy of our use of atomic wave functions rather than separated orbitals to represent s- and p-like states.

The absorptive part of the off diagonal elements of the conductivity tensor can be determined from measurements of the ferromagnetic Kerr effect: plane-polarized light reflected from a magnetized ferromagnetic metal becomes elliptically polarized with its major axis rotated from the original direction of polarization. Macroscopically, the rotation angle can be related to the absorptive part of the off diagonal elements of the conductivity tensor through Maxwell's field equations. The detailed
derivation is presented in Appendix B. This effect involves spin orbit coupling in an essential way. Previous calculations have been based on perturbation theory and simple models of the band structure. A major conflict developed between the results of different measurements. However, more recent work has tended to confirm, in a general way, the results of Krinchik and collaborators.

We have calculated the off diagonal element \( \sigma_{xy} \) of the conductivity tensor. Our results for \( \omega \text{Im}(\sigma_{xy}) \) are shown in Fig. XIX, where they are compared with results of Yoshino and Tanaka, Krinchik and Artemjev and Erskine and Stern. Our calculated results do not include any intraband contribution since the experimental data do not extend to low enough energies to permit determination of this quantity. Such a term would simply shift the calculated curves by a constant. The theoretical curves have the same general shape and order of magnitude as the experimental ones. However, the agreement in detail is not particularly good. The negative portion of \( \sigma_{xy} \) at low energy can be interpreted as indicating the dominance of transitions of minority spin electrons. The experimental curves become positive at a lower energy than the theoretical results. This is presumably a consequence of our overestimation of the exchange splitting. The negative peak at high energies is found, in our calculation to be displaced by about 1 eV with respect to the corresponding
experimental feature. A similar result was found for the diagonal elements of the conductivity and the explanation is probably the same. The smooth behavior of the experimental curves probably indicates the presence of substantial lifetime broadening.
CHAPTER IV
CONCLUSION

A self-consistent band structure for ferromagnetic nickel has been investigated using the tight binding method. The effects of exchange and spin-orbit interaction have been included. We believe that the comparison of the results of this calculation with experiment indicates that simple energy band theory employing a local exchange potential can successfully predict the essential features of the charge and magnetic moment distributions, momentum density, the Fermi surface, and of the optical properties of nickel. Although numerous discrepancies in detail exist, there is a large degree of general agreement between theory and experiment. There is no evidence for unexpectedly large many body effects, although some of the disagreement between theory and experiment may be due to our use of a simple, single particle approach. In view of the success of these calculations,\textsuperscript{11,105,106} and of our recent application to ferromagnetic iron,\textsuperscript{107} it seems that band theory should provide a basically satisfactory account of the properties of ferromagnetic nickel. The principal obstacles to such a conclusion concern observations of tunneling,\textsuperscript{108} and of spin polarized photo-emission\textsuperscript{109,110} which revealed that the spin polarization of electrons at energy $10^{-3}$ and 0.4-0.8 eV. below the
Fermi level is +11% and +15% respectively. The direction of the electron magnetic moments was found to be parallel to the magnetization. Based on oversimplified theories, it was interpreted as a measure of the spin polarization of the density of states. This indicated a contradiction with the results of band theory. It is possible, however, that detailed calculations of such phenomena based on band theory may remove much of the apparent disagreement.\textsuperscript{111,112} We hope to undertake this investigation.

This calculation can be improved in several ways. First, the variational freedom in the trial wave functions would be increased and the accuracy of the results improved if all the basis functions were chosen to be individual GTO. Some discrepancies in the Fermi surface and the optical properties have been shown in Chapter III as an indication of the inadequacy of our use of atomic wave functions rather than independent Gaussian orbitals to represent s and p-like states. Recently, the band structures of Li,\textsuperscript{113} Na,\textsuperscript{114} and Al\textsuperscript{115} have been investigated using basis functions consisting of individual GTO. Successful results were obtained after repeating the whole calculation several times with different sets of GTO. In principle, a basis set consists of individual Gaussian orbitals with large exponents that are capable of reproducing the atomic core states and one or two small exponents to allow sufficient variational freedom in the
conduction s and p-like states is more likely to give a satisfactory result. Of course those small exponents are subject to the restriction that the eigenvalues of the corresponding overlap matrices cannot be negative or unreasonably small.

A second modification which would be helpful is to include more conduction states, such as 4f for transition metals. The eigenfunctions are expected to be a better approximation to the exact solutions of the Schrödinger equation. The hybridization between the 4f and band states will undoubtedly improve our results of energy bands and conductivity tensor. In the conventional LCAO calculation, the problem may seem to be too complicated to be considered. The modification, made by Chaney and Dorman, to separate the variables in Cartesian coordinate and to take binomial expansions in the integrand drastically reduce the complexity of the problem. As a matter of fact, the integral program included in Appendix C is written in general that it can be used to calculate integrals between any pair of Gaussian orbitals.

Another possible improvement is to retain the angular dependence of the charge distribution when calculating the Xa exchange potential. This may effect the relative positions between the Fermi level and the X}_2 state of eg
symmetry as well as the unobserved $X_2$, hole pocket. The procedure involves three dimensional numerical integrations over rapidly oscillating functions which must be calculated with care. The cost in computer time, in this case, will be fairly high.
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TABLE I
Fourier Coefficients of the Coulomb and Exchange Potential and the Corresponding Corrections Resulting From Self-Consistency (in a.u.)

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<th>( \mathbf{K}^2 )</th>
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<th>( \Delta V_C (\mathbf{K}) )</th>
<th>( V_{x^+} (\mathbf{K}) )</th>
<th>( \Delta V_{x^+} (\mathbf{K}) )</th>
<th>( V_{x^+} (\mathbf{K}) )</th>
<th>( \Delta V_{x^+} (\mathbf{K}) )</th>
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Table I (cont'd)

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### TABLE II

Energy Difference for Selected States

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<tr>
<th>Majority Spin</th>
<th>Connolly^{15} ((\alpha=2/3))</th>
<th>Present ((\alpha=2/3))</th>
<th>Langlinais^{10} and Callaway ((\alpha=0.972))</th>
<th>Wakoh^{17} ((\alpha=1))</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\Gamma'<em>{12}-\Gamma'</em>{25})</td>
<td>0.478</td>
<td>0.483</td>
<td>0.506</td>
<td>0.488</td>
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<tr>
<td>(\Gamma_{25}'-\Gamma_{11}')</td>
<td>0.091</td>
<td>0.084</td>
<td>0.079</td>
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<tr>
<td>(X_5-X_1)</td>
<td>0.330</td>
<td>0.300</td>
<td>0.324</td>
<td>0.347</td>
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<tr>
<td>(X_5-X_2)</td>
<td>0.009</td>
<td>0.016</td>
<td>0.019</td>
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<tr>
<td>(X_5^*-X_5)</td>
<td>0.177</td>
<td>0.144</td>
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<td>(X_5'^*-X_1)</td>
<td>0.625</td>
<td>0.639</td>
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<td>(X_4'^*-X_1)</td>
<td>0.841</td>
<td>0.816</td>
<td>0.807</td>
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<td>(L_2'^*-L_{32})</td>
<td>0.036</td>
<td>0.016</td>
<td>-0.011</td>
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<tr>
<td>Minority Spin</td>
<td>Energy Difference for Selected States</td>
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<tr>
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<td>---------------------------------------</td>
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<tr>
<td>Connolly (*)=2/3</td>
<td>0.542 0.095 0.323 0.010 0.118 0.698 0.842</td>
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<tr>
<td>Present (a=2/3)</td>
<td>0.534 0.087 0.324 0.020 0.171 0.695 0.866</td>
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<td>Langlinais and Callaway (a=0.972)</td>
<td>0.544 0.083 0.372 0.020 0.171 0.372</td>
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<td>Wakoh (a=1)</td>
<td>0.535 0.086 0.695 0.047 0.029 0.024</td>
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TABLE III
Exchange Splitting of Certain States
at Symmetry Points (in Ry)

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<th></th>
<th>Present (α=2/3)</th>
<th>Langlinais and Callaway (α=0.972)</th>
<th>Wakoh (α=1)</th>
<th>Connolly (α=2/3)</th>
</tr>
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<tbody>
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<td>( \Gamma_1 )</td>
<td>0.001</td>
<td>0.022</td>
<td>0.018</td>
<td>-0.004</td>
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<td>( \Gamma_{25} )</td>
<td>0.052</td>
<td>0.060</td>
<td>0.067</td>
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<tr>
<td>( \Gamma_{12} )</td>
<td>0.057</td>
<td>0.063</td>
<td>0.071</td>
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<tr>
<td>( X_1 )</td>
<td>0.038</td>
<td>0.049</td>
<td>0.049</td>
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<td>( X_3 )</td>
<td>0.044</td>
<td>0.054</td>
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<td>( X_2 )</td>
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<td>( X_5 )</td>
<td>0.060</td>
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<td>( X_4' )</td>
<td>0.001</td>
<td>0.023</td>
<td>0.019</td>
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<tr>
<td>( L_1 )</td>
<td>0.030</td>
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<td>0.048</td>
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<tr>
<td>( L_{31} )</td>
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<td>0.060</td>
<td>0.066</td>
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<tr>
<td>( L_{32} )</td>
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<td>0.074</td>
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<tr>
<td>( L_2' )</td>
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<td>0.020</td>
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<table>
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<th>$\Gamma'(000)$</th>
<th>X(100)</th>
<th>X(001)</th>
<th>L($^{1/2}_{1/2}$)</th>
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<td>-0.3408 ($\Gamma_{12}^+$)</td>
<td>-0.2149 ($X_5^+$)</td>
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Table IV (cont'd)

Energy Levels at Symmetry Points (Ry)

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<th>K(3/4, 3/4, 0)</th>
<th>K(3/4, 0, 3/4)</th>
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TABLE V
Charge Density in Three Principle Directions (in a.u.)

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TABLE VI

Atomic Scattering Form Factors (in a.u.)

\[
\begin{array}{cccccc}
  \frac{K(2\pi)}{a} & \sin \frac{\theta}{\lambda} (\text{A}^{-1}) & \rho_{\text{band}}(K) & \rho_{\text{core}}(K) & \rho_{\text{total}}(K) & \rho_{\text{exp}}(K) \\
(1, 1, 1) & 0.2463 & 4.7865 & 15.5905 & 20.3769 & 20.10^{+0.16} \\
(2, 0, 0) & 0.2846 & 4.0977 & 14.9348 & 19.0325 & 18.55^{+0.16} \\
(2, 2, 0) & 0.4022 & 2.5201 & 12.8435 & 15.3636 & 15.34^{+0.12} \\
(3, 1, 1) & 0.4717 & 1.8478 & 11.6908 & 13.5386 & 11.18^{+0.11} \\
(2, 2, 2) & 0.4926 & 1.6683 & 11.3655 & 13.0338 & 8.74^{+0.09} \\
(4, 0, 0) & 0.5689 & 1.1514 & 10.2906 & 11.4420 & 8.73^{+0.09} \\
(3, 3, 1) & 0.6199 & 0.8324 & 9.6686 & 10.5010 \\
(4, 2, 0) & 0.6360 & 0.7690 & 9.4885 & 10.2575 \\
(4, 2, 2) & 0.6967 & 0.5123 & 8.8753 & 9.3875 \\
(3, 3, 3) & 0.7390 & 0.3659 & 8.5054 & 8.8713 \\
(5, 1, 1) & 0.7390 & 0.4030 & 8.5055 & 8.9084 \\
(4, 4, 0) & 0.8045 & 0.2143 & 8.0121 & 8.2264 \\
(5, 3, 1) & 0.8414 & 0.1497 & 7.7713 & 7.9210 \\
(6, 0, 0) & 0.8533 & 0.1616 & 7.6982 & 7.8598 \\
(4, 4, 2) & 0.8533 & 0.1173 & 7.6982 & 7.8155 \\
(6, 2, 0) & 0.8994 & 0.0807 & 7.4355 & 7.5161 \\
(5, 3, 3) & 0.9326 & 0.0129 & 7.2640 & 7.2769 \\
(6, 2, 2) & 0.9433 & 0.0207 & 7.2108 & 7.2315 \\
(4, 4, 4) & 0.9853 & -0.0417 & 7.0146 & 6.9730 \\
(5, 5, 1) & 1.0156 & -0.0527 & 6.8821 & 6.8294 \\
(7, 1, 1) & 1.0156 & -0.0211 & 6.8822 & 6.8610 \\
(6, 4, 0) & 1.0255 & -0.0522 & 6.8403 & 6.7881 \\
(6, 4, 2) & 1.0642 & -0.0770 & 6.6824 & 6.6054 \\
(7, 3, 1) & 1.0924 & -0.0735 & 6.5727 & 6.4992 \\
(5, 5, 3) & 1.0924 & -0.0958 & 6.5727 & 6.4769 \\
(8, 0, 0) & 1.1377 & -0.0675 & 6.4026 & 6.3351 \\
(7, 3, 3) & 1.1641 & -0.1003 & 6.3068 & 6.2065 \\
(8, 2, 0) & 1.1727 & -0.0812 & 6.2757 & 6.1945 \\
(6, 4, 4) & 1.1727 & -0.1129 & 6.2757 & 6.1629 \\
(8, 2, 2) & 1.2067 & -0.0907 & 6.1553 & 6.0646 \\
(6, 6, 0) & 1.2067 & -0.1091 & 6.1553 & 6.0461 \\
(7, 5, 1) & 1.2316 & -0.1077 & 6.0685 & 5.9608 \\
(5, 5, 5) & 1.2316 & -0.1200 & 6.0684 & 5.9484 \\
(6, 6, 2) & 1.2398 & -0.1130 & 6.0401 & 5.9272 \\
\end{array}
\]
TABLE VII
Magnetic Scattering Form Factors

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<th>\sin \frac{\theta}{\lambda} (Q^{-1})</th>
<th>\rho_{\text{spin}} (k)</th>
<th>\rho_{\text{core}} (k)</th>
<th>f (k)</th>
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### TABLE VIII
Spin Density in Three Principal Directions

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Compton Profiles

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### Table XI

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Table XI. Comparison of \( X \) hole pocket dimensions in atomic units. Numbers underlined are dimensions in the plane normal to the applied magnetic field. These dimensions contribute to the observed dHvA areas.
### TABLE XII

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<th>Hodges et al\textsuperscript{19}</th>
<th>Tsui\textsuperscript{80}</th>
<th>Stark\textsuperscript{81}</th>
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<td>(001) 0.089</td>
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Table XII. Extremal areas of Fermi surface cross sections in atomic units.

Refer to Fig. XIV for designations.
TABLE XIII

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<th>Present Results</th>
<th>Zornberg(^{10}) Parameter Set IV</th>
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Table XIII. Effective mass associated with Fermi surface portions. Refer to Fig. XIV for designations.
TABLE XIV

Interband Optical Conductivity Tensor (τ = ∞)

and the Joint Density of States

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<th>σ_{zz} (10^{15} \text{ sec}^{-1})</th>
<th>σ_{xy} (10^{14} \text{ sec}^{-1})</th>
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FIGURE CAPTIONS

Figure I  Coordinates for the evaluation of three-center integrals.

Figure II  Band structure for majority-spin states along certain symmetry directions.

Figure III  Band structure for minority-spin states along certain symmetric directions.

Figure IV  Band structure of nickel along some symmetry lines in the Brillouin zone. The effects of spin orbit coupling are included. States are labelled according to the symmetry of the largest spin component. The solid lines indicate states of minority spin, the dashed lines of majority spin. The horizontal line at -0.239 Ry. indicates the position of the Fermi energy.

Figure V  Band electrons (3d, 4s-p) charge density along three principle directions. Solid lines indicates the [100] direction, long dashes, the [110] direction, and dotted line, the [111] direction. The spherical average atomic charge density in 3d^8 4s^2 configuration is shown as short dashes.

Figure VI  Comparison of calculated and observed magnetic scattering form factors.
Figure VII  Spin density in three principle directions. Notation is the same as in Figure V.

Figure VIII Compton profile $J_k^\chi(q)$ for nickel. The (---) line is the core ($2s^2, 3s^2, 2p^6, 3p^6$) contribution. The other curves include the occupied band electrons and pertain to the following directions: long dashes, [100]; short dashes [111]; and solid curve, [110].

Figure IX Comparison of calculated and observed anisotropy in Compton profile. The solid curves are the present results and the long dashes are the experimental measurements of Eisenberger and Reed.\textsuperscript{71}

Figure X Comparison of the spherical averaged Compton profile with $\gamma$-rays Compton scattering measurements. The solid curves are the present results. The contribution from atomic $1s$ wave function has been included. Experimental results of Eisenberger and Reed\textsuperscript{71} and Manninen and Paakkari\textsuperscript{72} are shown as closed and open circles respectively. The dashed curve is the contribution from occupied (3d, 4s-p) band states. Corresponding experimental results are shown as $\Delta$, Ref. 71 and $\Lambda$ Ref. 72. Typical
experimental uncertainties are indicated by the error bars.

Figure XI  Projected density of states for majority spin.

Figure XII  Projected density of states for minority spin.

Figure XIII  Total density of states.

Figure XIV  Fermi surface cross sections in the (100) plane. The solid and short dashed curves are our results. A solid line indicates that states are predominately \( i \) minority spin, the short dashed line indicates majority \( (\uparrow) \) spin. The open circles, triangles, and squares are the experimental results of R. W. Stark.  The long dashed lines are obtained from an empirical formula given by Tsui.  The sheet (a) is the \( X_5 \) pocket, (b) is the \( X_2 \) pocket, (c) is the \( \Gamma \)-centered \( d^+ \) sheet, (d) is the large \( (sp^+) \) square, (e) is the small \( (sp^+) \) square.

Figure XV  Fermi surface cross sections in the (110) plane. The notation is the same as in Figure XIV. Note that the \( s-p^+ \) neck at \( L \) merges into the large \( d^+ \) sheet.

Figure XVI  Joint density of states.

Figure XVII  The real part of the \( xx \) component of the
conductivity tensor from 0 to 1.2 eV. Long dashes indicate the empirical Drude term (Eq. (3.32)); solid curve, the interband contribution in "sharp" limit, plus the Drude contribution, dashed curve, the interband contribution with $(\hbar/\tau=0.06 \text{ eV})$ plus the Drude contribution. Experimental results are shown as follows: □, Stoll\textsuperscript{86}; ◇, Shiga and Pells\textsuperscript{88}; ◆, Lynch et al.\textsuperscript{87}; ▲, Johnson and Christy\textsuperscript{91}; ○, Sasovskaya and Naskov\textsuperscript{90}; ●, Kirillora.\textsuperscript{89}

**Figure XVIII** The real part of $\sigma_{xx}$ from 1.0 to 6.0 eV. Notation is the same as in Figure VII.

**Figure XIX** The imaginary part of $\sigma_{xy}$ from 0 to 6 eV. The solid curve is the interband conductivity in the "sharp" limit; the short dashed curve is the conductivity calculated with $\hbar/\tau=0.06 \text{ eV}$. Experimental results are shown as follows: long dashed line, Erskine and Stern\textsuperscript{103}; ●, Yoshino and Tanaka\textsuperscript{99}; ○, Krinchik and Artemjev.\textsuperscript{101}
Figure I
Figure III
Figure IV

\[ \bar{k} \text{ IN UNITS OF } 2\pi/a \]
OCCUPIED BAND STATES CHARGE DENSITY (a.u.)
Figure VI
MAGNETIC MOMENT DENSITY

Figure VII
Figure VIII

Graph showing $J_k(q)$ vs $q(\text{au})$ for Ni, with different curves for different orbitals and the core configuration $(2s^2, 3s^2, 2p^6, 3p^6)$. The curves are labeled as follows:
- [1,0,0]
- [1,1,0]
- [1,1,1]
- Core

The x-axis represents $q(\text{au})$ ranging from 0 to 600, and the y-axis represents $J_k(q)$ ranging from 0 to 600.
Figure IX
Figure XI

DENSITY OF STATES (ELECTRONS/ATOM Ry)

MAJORITY SPIN

ENERGY (Ry)

Figure XI
Figure XII

DENSITY OF STATES (ELECTRONS/ATOM Ry)

ENERGY (Ry)

MINORITY SPIN

E_F
DENSITY OF STATES (ELECTRONS/ATOM Ry) vs. ENERGY (Ry)

BOTH SPINS

Figure XIII
Figure XIV
Figure XV
Figure XVII

Re $\sigma_{xx}(\omega)$ ($10^5$ sec$^{-1}$) vs. ENERGY (eV)
Figure XVIII

Re $\sigma_{xx}$ ($\omega$) (10^3 sec$^{-1}$)

ENERGY (eV)

1.0 1.4 1.8 2.2 2.6 3.0 3.4 3.8 4.2 4.6 5.0 5.4 5.8

120 200 280 360 440 520 600 680
Figure XIX
APPENDIX A

The Fourier Transform of Gaussian Orbitals

In the calculation of Compton profile, it is necessary to evaluate the Fourier transforms of atomic functions

\[ \chi_i(p) = \frac{1}{\sqrt{\Omega}} \int e^{-i\mathbf{p} \cdot \mathbf{r}} u_i(r) \, d^3r \]  

(3.10)

where \( \Omega \) is the volume of a unit cell and the atomic functions are expanded in terms of Gaussian orbitals of the type

\[ \frac{1}{\sqrt{4\pi}} e^{-\alpha r^2}; \sqrt{\frac{3}{4\pi}} x e^{-\alpha r^2}; \sqrt{\frac{15}{4\pi}} xy e^{-\alpha r^2}, \text{etc.} \]

according to different atomic symmetry, \( s, p, d \). Additional normalization constants from the radial part of the wave functions must be included (see Eqs. (2.13) and (2.15)). The Fourier transforms of these functions are tabulated below

S-functions

\[ \chi_S(p) = \frac{1}{\sqrt{4\pi\Omega}} \left( \frac{\pi}{\alpha} \right)^{3/2} e^{-\frac{p^2}{4\alpha}} \]  

(A.1a)
P-functions

\[ \begin{align*}
\chi_x(p) & = -\frac{i}{2} \sqrt{\frac{3}{4\pi \Omega}} \frac{1}{\alpha} \left( \frac{\pi}{\alpha} \right)^{3/2} e^{-\frac{p^2}{4\alpha}} \\
\chi_y(p) & = -\frac{i}{2} \sqrt{\frac{3}{4\pi \Omega}} \frac{1}{\alpha} \left( \frac{\pi}{\alpha} \right)^{3/2} e^{-\frac{p^2}{4\alpha}} \\
\chi_z(p) & = -\frac{i}{2} \sqrt{\frac{3}{4\pi \Omega}} \frac{1}{\alpha} \left( \frac{\pi}{\alpha} \right)^{3/2} e^{-\frac{p^2}{4\alpha}}
\end{align*} \]

\[ \begin{array}{c|c}
p_x \\
p_y \\
p_z
\end{array} \]  

\[ \text{(A.1b)} \]

D-functions

\[ \begin{align*}
\chi_{xy}(p) & = -\frac{1}{4} \sqrt{\frac{15}{4\pi \Omega}} \frac{1}{\alpha^2} \left( \frac{\pi}{\alpha} \right)^{3/2} e^{-\frac{p^2}{4\alpha}} \\
\chi_{yx}(p) & = -\frac{1}{4} \sqrt{\frac{15}{4\pi \Omega}} \frac{1}{\alpha^2} \left( \frac{\pi}{\alpha} \right)^{3/2} e^{-\frac{p^2}{4\alpha}} \\
\chi_{zx}(p) & = -\frac{1}{4} \sqrt{\frac{15}{4\pi \Omega}} \frac{1}{\alpha^2} \left( \frac{\pi}{\alpha} \right)^{3/2} e^{-\frac{p^2}{4\alpha}} \\
\chi_{yz}(p) & = -\frac{1}{4} \sqrt{\frac{15}{4\pi \Omega}} \frac{1}{\alpha^2} \left( \frac{\pi}{\alpha} \right)^{3/2} e^{-\frac{p^2}{4\alpha}} \\
\chi_{x^2-y^2}(p) & = -\frac{1}{4} \sqrt{\frac{15}{4\pi \Omega}} \frac{1}{\alpha^2} \left( \frac{\pi}{\alpha} \right)^{3/2} e^{-\frac{p^2}{4\alpha}} \\
\chi_{z^2-y^2}(p) & = -\frac{1}{4} \sqrt{\frac{15}{4\pi \Omega}} \frac{1}{\alpha^2} \left( \frac{\pi}{\alpha} \right)^{3/2} e^{-\frac{p^2}{4\alpha}}
\end{align*} \]

\[ \begin{array}{c|c|c|c|c|c}
p_x p_y \\
p_x p_z \\
p_y p_x \\
p_z p_x \\
\frac{1}{2\sqrt{3}} (3p_z^2 - p_x^2 - p_y^2)
\end{array} \]  

\[ \text{(A.1c)} \]
APPENDIX B

Ferromagnetic Kerr Effect

In Chapter III, Section E we compared the absorptive part of the off-diagonal elements of the conductivity tensor $\text{Im}[\sigma_{xy}(\omega)]$ with the results obtained from the magneto-optical measurements. In this appendix we shall examine the formal relationship between $\sigma(\omega)$ and the Kerr rotation angle.\textsuperscript{94,95} Consider a time dependent electric field

$$\mathbf{E}(t) = \frac{1}{\sqrt{2\pi}} \int \mathbf{E}(\omega) e^{-i\omega t} d\omega$$  \hspace{1cm} (A.2)

In the optical and infrared region the wave vector is effectively zero. The induced current takes the following form

$$\mathbf{j}(t) = \frac{1}{\sqrt{2\pi}} \int \mathbf{\chi}(t,t') \mathbf{E}(t') dt'$$  \hspace{1cm} (A.3)

For a homogeneous medium the conductivity is invariant under displacement of time, $\mathbf{\chi}(t,t') = \mathbf{\chi}(t-t')$. The Fourier transform of Eq. (A.3) can be written as

$$\mathbf{j}(\omega) = \sigma(\omega) \mathbf{E}(\omega)$$  \hspace{1cm} (A.4)

in the case of a cubic crystal with electron spin
quantized along the z-axis the conductivity tensor can be shown to be

\[
\Sigma(\omega) = \begin{pmatrix}
\Sigma_{xx} & \Sigma_{xy} & 0 \\
-\Sigma_{xy} & \Sigma_{xx} & 0 \\
0 & 0 & \Sigma_{zz}
\end{pmatrix}
\]  

(A.5)

As a result of broken symmetry by the spin orbit interaction the off diagonal elements \( \Sigma_{xy} \) are nonzero. For convenience we shall consider the incident plane wave as superposition of equal amplitude right and left circularly polarized light.

\[
E_\gamma = E(\omega) (\hat{x} + i\hat{y}) e^{-i\omega t}
\]  

(A.6)

where \( \hat{x} \) and \( \hat{y} \) are unit vectors along x and y directions respectively. In a similar manner, we define the RCP and LCP currents as

\[
J_\gamma = J(\omega) (\hat{x} + iy) e^{-i\omega t}
\]  

(A.7)

The corresponding conductivity which satisfies the relation

\[
J_\gamma = \nabla \cdot E_\gamma
\]  

(A.8)

is a simple scalar.
Maxwell's field equations then relate the complex index of refraction \((n + i\kappa)\) for RCP and LCP electric fields to the complex conductivity

\[
(n + i\kappa) = 1 + i\frac{4\pi\sigma}{\omega} \quad (A.10)
\]

In the case of light normally incident from vacuum

\[
\frac{E_{\text{reflected}}}{E_{\text{incident}}} = e^{i\theta} = \frac{(n + i\kappa) - 1}{(n + i\kappa) + 1} \quad (A.11)
\]

where \(\theta\) is the phase change of the reflected light and the sign convention is that for polarization along the plane of incidence. Denoting

\[
\Delta \theta = \theta_r - \theta_l \quad \Delta n = n_r - n_l \quad \Delta \kappa = \kappa_r - \kappa_l \quad (A.12)
\]

it can be shown that to the first order in these changes

\[
\frac{i}{2} = \frac{2i(\Delta n + i\Delta \kappa)}{[(n + i\nu)^2 - 1]} \quad (A.13)
\]

Similarly from Eqs. \((A.10)\) and \((A.9)\) one obtains

\[
n + i\nu = \frac{i2\pi\Delta \theta}{(n + i\nu)\omega} + \frac{-4\pi\nu nxy}{(n + i\nu)\omega} \quad (A.14)
\]
Eq. (A.14) was substituted into Eq. (A.13)

\[ \Delta \mu = \frac{-i 8\pi \phi_{xy}}{\omega(n+i\kappa)((n+i\kappa)^2-1)} \]  
\hfill (A.15)

The major axis of the elliptically polarized reflected light is rotated from the plane of polarization by an angle

\[ \frac{\Delta \mu}{2} = \text{Re} \left[ \frac{-i 4\pi \phi_{xy}}{\omega(n+i\kappa)((n+i\kappa)^2-1)} \right] \]  
\hfill (A.16)

Eq. (A.16) is the constant for the Magneto Kerr effect which is positive for rotation from x- to y-axis but it must be kept in mind that the reflected beam is traveling along the -z direction and Eq. (A.16) is valid for small values of \( n, \kappa, \) and \( \Delta \mu \) only.
APPENDIX C

LIST OF PROGRAMS

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<th>Program</th>
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<tr>
<td>1. Fourier coefficients of the Coulomb and exchange potential</td>
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<td>3. The integrals of $\alpha \cos(\alpha \hat{k} \cdot \hat{R})$ where $\alpha$ generates the star of $\hat{k}$</td>
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<td>4. Sum over direct lattice vectors for Hamiltonian overlap and momentum matrices</td>
<td>164</td>
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<tr>
<td>5. Bloch basis functions along three principle directions</td>
<td>174</td>
</tr>
<tr>
<td>6. Self-consistency</td>
<td>179</td>
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<tr>
<td>7. The central cell integrals of the spin-orbit coupling (p-p and d-d blocks)</td>
<td>190</td>
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<tr>
<td>8. Energy bands including the effects of spin orbit coupling</td>
<td>197</td>
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<tr>
<td>9. The momentum matrices between band states</td>
<td>201</td>
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<tr>
<td>10. The density of states</td>
<td>204</td>
</tr>
<tr>
<td>11. The interband optical conductivity tensor</td>
<td>211</td>
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<tr>
<td>12. The Compton profile</td>
<td>216</td>
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<td>GNBPT</td>
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<td>GNDPUM</td>
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<td>GWTGAS</td>
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PROGRAM 1. FOURIER COEFFICIENTS OF THE COULOMB AND EXCHANGE POTENTIAL

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CALCULATION OF THE FOURIER COEFFICIENTS OF POTENTIALS

SLATER TYPE WAVE FUNCTIONS ARE USED IN THIS PROGRAM

SC IDCUB=1, BCC IDCUB=2, FCC IDCUB=4

A=LATTICE CONSTANT (IN A. U. )

IGRLV=0, V(K) IS GENERATED IN ORDER OF INCREASING K**2

IGRLV=1, FOURIER COEFFICIENTS OF THE CHARGE DENSITY FOR BOTH SPINS ARE GENERATED IN ORDER OF K VECTORS

IF(ISORT.NF.0) K IS SORTED IN ORDER OF INCREASING MAGNITUDE

NKPT IS THE DIMENSION OF THE RECIPROCAL LATTICE VECTORS KXX(I) ECT.

MAXK2=THE SQUARE OF THE MAXIMUM MAGNITUDE OF THE RECIPROCAL LATTICE VECTORS GENERATED

IDIM IS THE DIMENSION OF THE DIRECT LATTICE VECTORS

MAXR2=THE SQUARE OF THE MAXIMUM MAGNITUDE OF THE DIRECT LATTICE VECTORS

NSTA IS THE NUMBER OF ATOMIC STATES CONSIDERED, MAXIMUM=7

C(I,J) IS THE J'S COEFFICIENT OF THE I'S WAVE FUNCTION

FX(I,J) IS THE J'S EXPONENTS OF THE I'S WAVE FUNCTION

NOR(I) IS THE NUMBER OF ORBITALS IN THE I'S WAVE FUNCTION

IB(I,J) IS THE ORBITAL IDENTIFICATION OF THE I'S WAVE FUNCTION

CHARGE(I) IS THE NUMBER OF ELECTRONS IN THE I'S STATE

EXCH(I) IS DENSITY=0.333 AT POINT R(I)

* * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *

IMPLICIT REAL*8(A-F,H,O-Z)
INTEGRAL*2 KKX,KKY,KKZ,NB,XX,YY,KZ,NNB
DIMENSION AX(400),AY(400),AZ(400),Y(100)
DIMENSION KSQ(500)
COMMON/CHARGE/CHARGE(7),CHARUP(7),CHARDN(7)
COMMON/VKO/C(7,11),EX(7,11),FACTO(10),IB(7,11),NORB(7),NSTA
COMMON/EXCH/R(96),EXCH(96),EXUP(96),EXDN(96)
COMMON/CONST/A,R0,PI,OMETHD
COMMON/LCS/KXX(500),KKY(500),KKZ(500),NB(500)
PI=3.141592653589793D0
ONETHO=1.00/3.D0
FACTO(1)=1.D0
DO 11 I=2,10
11 FACTO(I)=FACTO(I-1)*DFLOAT(I)
READ(5,3) A,IDCUB,NKPT,MAXK2,IDIM,MAXR2,KPTPRT,NSTA,IGRLV,ISORT,
& IPUN
3 FORMAT(F10.5,1C15)
AAA=A*A*A
AKR=2.*D0*PI/A
OMFGA=AAA/DFLOAT(IDCUB)
AHALF=A/2.*D0
IF(IDCUB.EQ.1) A=HALF=A

DEFINE R AND WEIGHT FACTOR FOR 96 POINTS GAUSSIAN INTEGRATION IN THE
WIGNER SEITZ CELL

RO3=3.00/(4.00*PI)*OMEGA
RO=RO3*ONETHD
CALL GTGAS(96,Y,R,W)
DO 54 I=1,96
54 R(I)=RO*(R(I)+1.00)/2.00

RENORMALIZATION OF THE WAVE FUNCTION

2 FORMAT(15,2F10.5)
1 FORMAT(3A4,8X,15,2F10.5)
ELECT=0.00
FMAG=0.00
DO 12 I=1,NSTA
READ(5,1) Z1,Z2,Z3,NORB(I),CHARUP(I),CHARDN(I)
ELEUP=ELEUP+CHARUP(I)
ELEDN=ELEDN+CHARDN(I)
CHARGE(I)=CHARUP(I)+CHARDN(I)
WRITE(6,12) Z1,Z2,Z3,NORB(I),CHARUP(I),CHARDN(I),CHARGE(I)
NN=NORB(I)
DO 15 J=1,NN
READ(5,2) IB(I,J),EX(I,J),C(I,J)
4 FORMAT(1X,*L='F10.5,'*F5.5X,*F10.5,'*F5.5X,*F10.5)
WRITE(6,4) IB(I,J),EX(I,J),C(I,J)
AJ=IB(I,J)
II=2*IB(I,J)
TWOZ=(2.00*EX(I,J))**(AJ+0.5)
15 C(I,J)=C(I,J)*TWOZ/DSQRT(FACTO(I))
10 CONTINUE
ELECT=ELEUP+ELEDN
EMAG=ELEUP-ELEDN

GENERATE PERMUTED DIRECT LATTICE VECTORS

IDC=8/IDCUB
IF(IDCUB.EQ.1) IDC=1
CALL GPERMK(KKX,KKY,KKZ,KSO,IDIM,IDC,MAXR2,0)
DO 31 II=1,IDIM
\[ AX(I) = \text{AHALF} \times KKX(I) \]
\[ AY(I) = \text{AHALF} \times KKY(I) \]
\[ AZ(I) = \text{AHALF} \times KKZ(I) \]

CALL SVKO(VK0)

CO1 = ELECT \times PI \times 8.0

CECH = -9.0 / RO3 \times (3.0 / PI)^{N} \times \text{ONETHD} \times RO / 2.0

CEFE = -9.0 / RO3 \times (6.0 / PI)^{N} \times \text{ONETHD} \times RO / 2.0

WRITE(6, 50) A, RO, ELECT, EMAG, IDCUB, NKPT, MAXK2, IDIM, MAXR2, NSTA, IGR

&ISORT

PRINT 51

INDEPENDENT DIRECTIONS USED TO CALCULATE THE SPHERICALLY AVERAGED CHARGE DENSITY ARE READ IN SUBROUTINE SEXCH

CALL SEXCH(AX, AY, AZ, IDIM)

PUNCH THE DENSITY AS INPUT TO THE SELF-CONSISTENCE PROGRAM

34 FORMAT(5D15.8)

DO 33 KR = 1, 96

IF(IPUN.NE.0) WRITE(7, 34) R(KR), W(KR), EXCH(KR), EXUP(KR), EXDN(KR)

EXCH(KR) = EXCH(KR)^{N} \times \text{ONETHD}

EXUP(KR) = EXUP(KR)^{N} \times \text{ONETHD}

EXDN(KR) = EXDN(KR)^{N} \times \text{ONETHD}

33 CONTINUE

PRINT 51

51 FORMAT(1H1)

IF(IGRLV.NE.0) PRINT 55

55 FORMAT(3X,'K2',5X,'Coulomb(K)',7X,'EXCHANGE(K)',7X,'EXCH UP(K)',17X,'EXCH DOWN(K)',/)

IF(IGRLV.NE.0) PRINT 56

56 FORMAT(3X,'K2',5X,'Coulomb(K)',7X,'EXCHANGE(K)',7X,'EXCH UP(K)',17X,'EXCH DOWN(K)',8X,'DEN UP(K)',8X,'DEN DOWN(K)',6X,'KX',3X,'KY',23X,'KZ',2X,'NO',/)

GENERATE INDEPENDENT RECIPROCAL LATTICE VECTORS.

IF(IGRLV.NE.0) CALL GINDPK(KKX, KKZ, KSQ, NKPT, IDCUB, MAXK2, NB, 1, ISORT)

KINCM = 1

IF(IGRLV.EQ.0.AND.IDCUB.EQ.2) KINCM = 2

K2 = 1

DO 999 NPT = 1, NKPT, KINCM

IF(IGRLV.EQ.0) GO TO 21

KX = KKX(NPT)

KY = KKZ(NPT)
KZ=KKZ(NPT)
NNB=NN(NPT)
  IF(K2.EQ.KSQ(NPT)) GO TO 99
  K2=KSQ(NPT)
  GO TO 22
21  K2=NPT-1
22  CONTINUE
  RK2 = OFLOAT(K2)
  RS=RK2*AKR*AKR
  RK = dsqrtcrs
  IF(K2.NE.0) GO TO 69
C    CALCULATE THE FOURIER COEFFICIENT V(K=0)
C
  VKX=0.DO
  VKUP=0.DO
  VKDN=0.DO
  DO 42 I=1,96
    VKUP=VKUP+EXUP(I)*R(I)**2
    VKDN=VKDN+EXDN(I)*R(I)**2
  42  VKX=VKX+EXCH(I)*R(I)**2
  VEXCH=CEXCH*VKX
  VEXUP=CEXFE*VKUP
  VEXDN=CEXFE*VKDN
  GEXCH=VEXCH
  GEXUP=VEXUP
  GEXDN=VEXDN
  VCoul=-4.DO*PI*VK0/3.DO/OMEGA
  GCoul=VCoul
  IF(IGRLV.EQ.0) GO TO 25
  GUMUP=ELEUP/OMEGA
  GUMDN=ELEDN/OMEGA
  IF(NPT.LE.KPTPRT) WRITE(6,7)K2,GCoul,GEXCH,GEXUP,GEXDN,GUMUP,GUMDN,
  EXXX,EXX,EXY,EXZ,NNB
  WRITE(1) K2,GCoul,GEXCH,GEXUP,GEXDN,GUMUP,GUMDN,KX,KY,KZ,NNB
  GO TO 999
25  CONTINUE
  IF(NPT.LE.KPTPRT) WRITE(6,7)K2,GCoul,GEXCH,GEXUP,GEXDN
  WRITE(1) GCoul,GEXCH,GEXUP,GEXDN,K2
  GO TO 999
C    CALCULATE THE FOURIER COEFFICIENTS OF THE EXCHANGE POTENTIAL BY 96 POINTS
C    GAUSSIAN INTEGRATION
C
69  CONTINUE
  VKX=0.DO
nkup=0.0,0
nkdn=0.0,0
41 do 44 i=1,96
  vkup=vkup+exup(i)*r(i)*w(i)*dsin(rk*r(i))
  vkdn=vkdn+exdn(i)*r(i)*w(i)*dsin(rk*r(i))
44 vks=vks+exch(i)*r(i)*w(i)*dsin(rk*r(i))
  vech=vech*vkx/rk
  vexup=vechfe*vkup/rk
  vexdn=vechfe*vkdn/rk
  gexch=vech
  gexup=vexup
  gexdn=vexdn
  if (igrvl,ne.,0) go to 101

calculate the fourier coefficients of the coulomb potential
fact=8.00*pi/rs/omega
sum=-co1/rs
call coulom(charge, sum, rs, fact)
gcoul=sum
23 if (npt,le.,kptprr) write (6,7) k2, gcoul, gexch, gexup, gexdn
write(1) gcoul, gexch, gexup, gexdn, k2
go to 999 101 continue

calculate the fourier coefficients of the charge densities for both spins
as input to the self-consistency program
fact=1.00/omega
sumup=0.0,0
sumdn=0.0,0
call coulom(charup, sumup, rs, fact)
call coulom(chardn, sumdn, rs, fact)
gumup=sumup
gumdn=sumdn
gcoul=(sumup+sumdn)*8.0,d*pi/rs
99 continue
if (npt,le.,kptprr) write (6,7) k2, gcoul, gexch, gexup, gexdn, gumup, gumdn,
  kx,ky,kz,nnb
write(1) k2, gcoul, gexch, gexup, gexdn, gumup, gumdn, kx,ky,kz,nnb
999 continue
7 format (15,6e18.8,5i5)
write (6,50) arr, elect, emag, idcub, nkpt, maxk2, idim, maxr2, nsta, igrlv
6, isort
50 format (1x,/,1x, 'lattice const= ', f10.5,3x,'r=' , f10.5,3x,'elect no=
  1', f7.2,3x,'mag no= ', f7.4,3x,'no atoms/lattice= ',15,/,1x,
2*NO=1,18,3X,*K2 MAX=1,15,3X,*R NO=1,18,3X,*R2 MAX=1,15,3X,*OPRT
3ALS NO=1,15,3X,*GEN RLV=1,12,3X,*SORT=1,12)
STOP
FN7
**PROGRAM 2, THE COULOMB, EXCHANGE, KINETIC, OVERLAP, & MOMENTUM INTEGRALS**

**CALCULATE INTEGRALS \langle G \mid i, R-A \rangle V(R) \rangle G \mid j, P \rangle**

**Gaussian type wave functions are used**

A = lattice constant (in a. u.)

SCO IDCUB = 1, BCCO IDCUB = 2, FCCO IDCUB = 4

EXPCVG = convergent critical DEXP(-EXPCVG) = 0.00

MXOBNO = no of symmetries considered = 3 FOR S, P, AND D functions

K2MAX = the square of the maximum magnitude of the reciprocal lattice vectors used

MAXA2 = the square of the maximum magnitude of the direct lattice vectors

NKPT = maximum no of reciprocal lattice vectors, dimension KXX(NKPT)

KREAD = no of Fourier coefficients read in (1)

DIMENSION FCS(NORDIM, NKDIM, NRDIM), FCS1(NORDIM, NKDIM)

IOBNO(L) = orbital number included for L-th symmetry

ALPHA = Gaussian exponential parameters

**IMPLICIT REAL *8 (A-F, H, O-Z)**

INTEGER*2 KKX(8184), KKY(8184), KKZ(8184), NB(8184), IX(100), IY(100), IZ(100)

DIMENSION SCOUL(125), SEXCH(125), SEXUP(125), SEXDN(125), SOVLP(7, 7, 7)

DIMENSION ALP(3,14), CN(3,14), CIJ(8, 8)

DIMENSION FCS1(7,100), FCS2(7,100), FCS3(7,100), FCS(7,100, 11)

DIMENSION SCO(4,14), PCD(3,11), OCD(1,5)

DIMENSION DV(5,5,5), GC(27), GX(27), GU(27), GO(27)

DIMENSION GWTSPD(3), IOBNO(3), KSQU(8184), ISQU(100)

COMMON/GFUC/AKR, W, DELT, WOB, DSTEP, MAXK, MAXR

COMMON/LCS/GCOUL(4801), GEXCH(4801), GEXUP(4801), GEXDN(4801)

DATA GWTSPD/*S', 'P', 'O'*/

1 FORMAT(A8,F10.5,F7.2)

READ(5,1) CRYSTAL, A, EXPCVG, IDCUB, MXOBNO, MAXA2, IADIM, K2MAXM, & NORDIM, NKDIM, NRDIM, NKPT, KREAD

PI = 3.141592653589793

ALPHA = A

DATA PI, A, AHALF, OMEGA/A)

**DEFINE GAUSSIAN EXPONENTS AND NORMALIZATION CONSTANTS**

4 FORMAT(9I5)

READ(5,4) (IOBNO(I), I=1, MXOBNO)

DO 10 NOB = 1, MXOBNO

ID = IOBNO(NOB)
DO 10 J=1,10
READ(5,15) ALPHA
ALP(NOB,J)=ALPHA
A2=ALPHA*2.00
AAA=(3.00*ALPHA/PI)**2.00/DSQRT(4.00*PI
A0=-0.50
DO 11 L=1,NOB
A0=A0+1.00
A1=DFLOAT(2*L-1)
11 AAA=AAA+DSQRT(A1*A2/A0)
CN(NOB,J)=AAA
10 WRITE(6,12) CRYSTL,J,GWTSPD(NOB),ALPHA,AAA
12 FORMAT(IX,A8,I4,A2,'FXPONENT=',F16.8,2X,'NORM=',E16.8)
15 FORMAT(F8.5,4D16.8)

DEFINE BINOMIAL EXPANSION COEFFICIENTS

CIJ(1,1)=1.00
CIJ(2,1)=1.00
CIJ(2,2)=1.00
DO 70 I=3,8
CIJ(I,1)=1.00
CIJ(I,1)=1.00
IM1=I-1
70 CIJ(I,J)=CIJ(IM1,J-1)+CIJ(IM1,J)

GENERATE INDEPENDENT DIRECT LATTICE VECTORS

IDC=1
IF(IDCUB,NE,1) IDC=B/IDCUB
CALL GINDPK(IX,IY,IZ,ISOU,IADIM,IDC,MAXA2,NB,0,1)
DO 60 I=1,IADIM
WRITE(6,4) I,IX(I),IY(I),IZ(I),ISOU(I)
60 CONTINUE

READ IN FOURIER COEFFICIENTS OF THE COULOMB AND EXCHANGE POTENTIAL

DO 23 J=1,KREAD
23 READ(I,END=22) GCOUL(J),GEXCH(J),GEXP(J),GEXDN(J),K2
22 CONTINUE

GENERATE INDEPENDENT RECIPROCAL LATTICE VECTORS AND THE PERMUTATION NUMBER

CALL GINDPK(KX,KY,KZ,KSQN,KPT,IDCUB,K2MAXM,NB,1,1)
WRITE(6,2) A,EXPCVG,IDCUB,MAXBND,MAXA2,IADIM,K2MAXM,KREAD,
&NOROIM,NKDIM,NRDIM,NKPT,(GWTSPO(I),IOBNO(I),I=1,MAXANO)
2 FORMAT(1X,'LATTICE CONST=',F10.5,3X,'CONVERGENT EXPO=',
  1F11.4,3X,'ATOMS/LATTICE=',I2,3X,'MAX N=',I5,3X,'MAX A2=',I5,3X,
  2'A0 M=',*I4,'/X,'MAX K2=',*I,16,'/X,'V(K) NO=',*I,16,'/X','DIM FCS(*,
  11,'*','*','*','*','*','*','*','*','*','*','*','*','*','3X,'NKPT=',*I,16,'/X','1X,4(A2,14,'ORBITAL NO=',*I,14,
  4'X,/)')
C
C CALCULATE INTEGERS BETWEEN ORBITALS OF ORDER NORDA AND NORDB WITH DIRECT
C LATTICE VECTORS FROM NRST TO NREND
C NORD OR NORDB=1 FOR S, 2 FOR P, AND 3 FOR D
999 READ(5,4,END=1000) NORDA,NORDA,NRST,NREND
31 FORMAT(1X,2A2,3X,'R=('2I5,2X)')
!R!TE(6.31) GWTSPO(NORDA),GWTSPO(NORDB),NRST,NREND
NORD=NORDA+NORDB-1
NR02=NORD+2
NOR3=NORD+3
IAOBNO=IOBNO(NORDA)
IBOBNO=IOBNO(NORDB)
M2MAX=IBOBNO
DO 101 M1=1,IAOBNO
  IF(IAOBNO.EQ.IBOBNO) M2MAX=M1
  DO 101 M2=1,M2MAX
  ALP1=ALP(NORDA,M1)
  ALP2=ALP(NORD3,M2)
  W=1.00/(ALP1+ALP2)
  ALAMDA=ALP1*ALP2*W
  DELT=DSQR(T(P1*W))
  U1=ALP1*W
  U2=ALP2*W
  DSTEP=U1*AHALF
  W04=W/4.00
  G=EXPVCVG/(AKR2*W04)
  IF(G,GT,K2MAX) G=K2MAXM
  MAXK2=G
  MAXK=SQRT(G)*2.0
  MAXR=DSQR(T(EXPVCVG/ALAMDA)/AHALF+2.0
  MR=SQRT(FLOAT(ISQU(NREND)))+1
  IF(MAXR.GT.MR) MAXR=MR
  CALL GINTFCIFC.S,NORD,NORD I,M,NKDIM,NRDIM!
DO 100 NRC=NRST,NREND
  AX=AHALF*I(X(NRC))
  AY=AHALF*I(Y(NRC))
  AZ=AHALF*I(Z(NRC))
  RAB2=AX*AX+AY*AY+AZ*AZ
  EXPAR=ALAMDA*RAB2
IF(EXPA.GT.EXPCVG) GO TO 1C1
RA8=DSQRTR(RAB2)
AZETA=DEXP(-FXPA)
ADX=-U2*AX
ADY=-U2*AY
ADZ=-U2*A
BDX=U1*AX
BDY=U1*AY
BDZ=U1*A
CONST=AZETA*CN(NORDA, M1)*CN(NORDB, M2)
DO 124 I=1,NORD3
SCOU(I)=0.D0
SEXCH(I)=0.D0
SEXUP(I)=0.D0
SEXDN(I)=0.D0
124 CONTINUE
DO 121 I1=1,NORD2
DO 121 I2=1,NORD2
DO 121 I3=1,NORD2
SOVLP(I1, I2, I3)=0.D0
121 CONTINUE
NRX=IX(NRC)+1
NRY=IY(NRC)+1
NRZ=IZ(NRC)+1
DO 127 I=1,NORD2
DO 127 K=1,MAXK
FCS1(I,K)=FCS(I,K,NRX)
FCS2(I,K)=FCS(I,K,NRY)
FCS3(I,K)=FCS(I,K,NRZ)
127 CONTINUE
SUM OVER RECIPROCAL LATTICE VECTORS
DO 105 K=1,NKPT
KS=K-SQUR(K)
GK2=(EXPCVG-EXPA)/(AKR2*W02)
IF(KS.GT.MAKXK2. OR. KS.GT. GK2) GO TO 1C6
K1=KKX(K)+1
K2=KKY(K)+1
K3=KKZ(K)+1
KK=KS+1
N=NB(K)
CD=DFLOAT(N)/6.D0
DO 111 I=1,NORD
S1=FCS1(I, K1)
S2=FCS1(I, K2)
DO 202 IB3=1,NORD2
DO 202 IB2=1,NORD2
DO 202 IB1=1,NORD2
IBT=IB1+IB2+IB3-2
IF (IBT.LT.NORD-2 .OR. IBT.GT.NORD) GO TO 202
TC=0.DO
TX=0.DO
TU=0.DO
TD=0.DO
TO=0.DO
CA1=1.DO
DO 211 NA1=1,IA1
JA1=IA1-NA1+1
CA2=C1J(IA1,JA1)
DO 212 NA2=1,IA2
JA2=IA2-NA2+1
CA3=C1J(IA2,JA2)
DO 213 NA3=1,IA3
JA3=IA3-NA3+1
CB1=C1J(IA3,JA3)
DO 221 NB1=1,IB1
JB1=IB1-NB1+1
NAB1=JA1+JB1-1
CB2=C1J(IB1,JB1)
DO 222 NB2=1,IB2
JB2=IB2-NB2+1
NAB2=JA2+JB2-1
CB3=C1J(IB2,JB2)
DO 223 NB3=1,IB3
JB3=IB3-NB3+1
NAB3=JA3+JB3-1
CA=C1J(IB3,JB3)*CA1*CA2*CA3*CB1*CB2*CB3
IF (IBT.NE.NORD) GO TO 225
NIJ=((NAB1-1)*NORD+NAB2-1)*NORD+NAB3
TC=TC+CA*SCOU(NIJ)
TX=TX+CA*SEXCH(NIJ)
TU=TU+CA*SEXUP(NIJ)
TD=TD+CA*SEXDN(NIJ)
225 TO=TO+CA*SVLP(NAB1,NAB2,NAB3)
CB3=CB3*BDZ
223 CONTINUE
CB2=CB2*BDY
222 CONTINUE
CB1=CB1*BDX
221 CONTINUE
CA3=CA3*BDZ
CA2 = CA2 * ADY
CA1 = CA1 * ADX

CONTINUE

IF (IBT .NE. NOEDB) GO TO 226
IB1J = IB1J + 1
GC(IB1J) = TC
GX(IB1J) = TX
GU(IB1J) = TU
GO(IB1J) = TD

CONTINUE

226 OV(IB1, IB2, IB3) = TO

CONTINUE

C CALCULATE KINETIC ENERGY AND MOMENTUM MATRICES FOS. (2.49A) AND (2.59)

IB1J = 0
DO 301 IB3 = 1, NOEDB
IB3M1 = IB3 - 1
IB3M2 = IB3 - 2
DO 301 IB2 = 1, NOEDB
IB2M1 = IB2 - 1
IB2M2 = IB2 - 2
DO 301 IB1 = 1, NOEDB
IB1M1 = IB1 - 1
IB1M2 = IB1 - 2
PX = -C1 * OV(IB1+1, IB2, IB3)
PY = -C1 * OV(IB1, IB2+1, IB3)
PZ = -C1 * OV(IB1, IB2, IB3+1)

IF (IB1M1 .GT. 0) PX = PX + DFLOAT(IB1M1) * OV(IB1M1, IB2, IB3)
IF (IB2M1 .GT. 0) PY = PY + DFLOAT(IB2M1) * OV(IB1, IB2M1, IB3)
IF (IB3M1 .GT. 0) PZ = PZ + DFLOAT(IB3M1) * OV(IB1, IB2, IB3M1)
AK = C1 * DFLOAT(2*IB1-1) * OV(IB1, IB2, IB3) - C2 * OV(IB1+2, IB2, IB3)

1 + C1 * DFLOAT(2*IB2-1) * OV(IB1, IB2, IB3) - C2 * OV(IB1, IB2, IB3+2)
2 + C1 * DFLOAT(2*IB3-1) * OV(IB1, IB2, IB3) - C2 * OV(IB1, IB2, IB3+2)

IF (IB1M2 .GT. 0) AK = AK - DFLOAT(IB1M2) * OV(IB1M2, IB2, IB3)
IF (IB2M2 .GT. 0) AK = AK - DFLOAT(IB2M2) * OV(IB1, IB2M2, IB3)
IF (IB3M2 .GT. 0) AK = AK - DFLOAT(IB3M2) * OV(IB1, IB2, IB3M2)

IB1J = IB1J + 1
GO = OV(IB1, IB2, IB3)
GK = AK
GPX = PX
GPY = PY
GPZ = PZ
```
WRITE(2) NRC, M1, M2, IJAB, GC(IBIJ), GX(IBIJ), GJ(IBIJ), GD(IBIJ), GK, GO,
& GPX, GPY, GPZ
WRITE(6, 300) M1, M2, NRC, KTDL, IJAB, IA1, IA3, IB1, IB2, IB3, GC(IBIJ),
& GX(IBIJ), GJ(IBIJ), GD(IBIJ), GK, GO, GPX, GPY, GPZ
301 CONTINUE
300 FORMAT(3I3, 15.13, 1X, 3I1, 3I1, 9(1X, E11.5))
201 CONTINUE
100 CONTINUE
101 CONTINUE
GO TO 999
1000 STOP
END
```
PROGRAM 3. THE INTEGRALS OF $\cos(\tau K\cdot R)$ WHERE $\tau$ GENERATES THE STAR OF $K$

PROGRAM 3. THE INTEGRALS OF $\cos(\tau K\cdot R)$ WHERE $\tau$ GENERATES THE STAR OF $K$

**CALCULATE** $\langle G(I,J,R-A) \mid \cos(K\cdot R) \mid G(J,R) \rangle$

**A** = LATTICE CONSTANT (IN A. U.)

**SC0, IDCUB** = 1, BCC; **IDCUB** = 2, FCC; **IDCUB** = 4

**EXPVCVG** = CONVERGENT CRITICAL DEXP(-EXPVCVG) = 0.00

**MAXOBNO** = NO OF SYMMETRIES CONSIDERED = 3 FOR S, P, AND D FUNCTIONS

**MAXK2** = THE SQUARE OF THE MAXIMUM MAGNITUDE OF THE RECIPROCAL LATTICE VECTORS

**NKPT** = MAXIMUM NO OF RECIPROCAL LATTICE VECTORS, DIMENSION $KKX(NKPT)$

**DIMENSION** FCS1(NORDIM, NRDIM) ECT.

**IMPLICIT** REAL *8 (A-F, H-O-Z)

**INTEGER** 2 NRC, M1, M2, IJAB

**INTEGER** 2 IX(200), IY(200), IZ(200)

**INTEGER** 2 KXX(300), KKY(300), KKZ(300), NB(300)

**DIMENSION** SIIJ(125)

**DIMENSION** ALP(3,14), CN(3,14), CIJ(8,8)

**DIMENSION** FCS1(7,20), FCS2(7,20), FCS3(7,20)

**DIMENSION** SCO(4,14), P(3,11), DCO(1,5)

**DIMENSION** GWTSRD(3), IOBNO(3)

**DIMENSION** KSOU(500), KSOU(200)

**COMMON/GSIJF/W.DELT, W04, DSTEP, MAXR**

**DATA GWTSRD/*S, P, D*/

1 **FORMAT** (A8,F10.5,F7.2,1015)

**READ** (5,1) CRYSTL,A,EXPCVG, IDCUB, MAXOBNO,MAXA2, IADIM, K2MAXM, NORDIM, NKPT, NRDIM

**PI** = 3.1415926535897930

**AKR** = 2.00*PI/A

**AKR2** = AKR**2

**AHALF** = A/2.00

IF(IDCUB.EQ.1) AHALF = A

**OMEGA** = A**3/DFloat(IDCUB)

4 **FORMAT** (915)

**DEFINE** GAUSSIAN EXPONENTS AND NORMALIZATION CONSTANTS

**READ** (5,4) (IOBNO(I), I=1, MAXOBNO)

**DO** 10 NOB=1, MAXOBNO

10 **ID** = IOBNO(NOB)

**DO** 10 J=1, ID

**READ** (5,15) ALPHA

**ALP**(NOB,J) = ALPHA

**A2** = ALPHA**2*2.00**
AAA=(8.00*ALPHA/PI)**0.2500/DSQRT(4.00*PI)
A0=-0.500
DO 11 L=1.NOB
    A0=A0+1.00
    A1=DFLOAT(2*L-1)
11 AAA=AAA*DSQRT(A1*A2/A0)
C(NOB,J)=AAA
10 WRITE(6,12) CRYSTL,J,GWTSPO(NOB),ALPHA,AAA
12 FORMAT(1X,A8,14.2,14.2,EXPONENT=1,F16.9,2X,NORM=1,E16.8)
15 FORMAT(F8.5,4D16.8)

DEFINE BINOMIAL EXPANSION COEFFICIENTS
CIJ(1,1)=1.00
CIJ(2,1)=1.00
CIJ(2,2)=1.00
DO 70 I=3,N
    CIJ(I,1)=1.00
    CIJ(I,1)=1.00
    IM1=I-1
    DO 70 J=2,IM1
70 CIJ(I,J)=CIJ(IM1,J-1)+CIJ(IM1,J)

GENERATE INDEPENDENT DIRECT LATTICE VECTORS
IDC=1
IF,IDCUB,NE,1) IDC=8,IDCUB
CALL GINDPK(IX,IY,IZ,ISQU,IADIM,IDC,MAXA2,NB,C,1)
DO 60 I=1,IADIM
    WRITE(6,4) I,IX(I),IY(I),IZ(I),ISQU(I)
60 CONTINUE

GENERATE INDEPENDENT RECIPROCAL LATTICE VEORS AND THE PERMUTATION NUMBER
CALL GINDPK(KXX,KKY,KKZ,KSOU,TKPT,IDCUB,K2MAXM,NB,1,1)
WRITE(6,2) A,EXPCCVG,IDCUB,MXOBNO,MAXA2,IADIM,K2MAXM,
&NORDIM,NRDIM,TKPT*(GWTSPO(1),10RNO(1),1=1,MXOBNO)
2 FORMAT(1X,LATTICE CONSTANT=1,F10.5,3X,EXP CONVERGENT=1,F10.5,
13X,ATOMS/LATTICE=1,v12,3X,MAX N=1,v15,3X,MAX A2=1,v15,3X,
2*A DIM=1,14//,1X,*MAX K2=1,v16,2X,*DIM FCS(1,
315,*,*),15,*),2X,*NKPT=1,v18,1X,4(A2,* ORBITAL NO=1,v14,5X),//)

CALCULATE INTEGERS BETWEEN ORBITALS OF ORDER NORDA AND NORDB WITH DIRECT
LATTICE VECTORS FROM NRSN TO NREND
NORDA OR NORDB=1 FOR S, 2 FOR P, AND 3 FOR D
READ(5,4,END=1000) NORDA,NORDB,NRST,NREND
31 FORMAT(1X,//,1X,2A2,3X,*R=('*,215,'*),//)
WRITE(6,31) GWTSPD(NORDA),GWTSPD(NORDA),NRST,NREND
NORD=NORDA+NORDB-1
NORD2=NORD+2
IA0BN0=IOBNO(NORDA)
1B0BN0=IOBNO(NORDB)
M2MAX=IBOBN0
CONTINUE
DO 105 K=1,NKPT
K5=KSQUC(K)
K1=KKX(K)
K2=KKY(K)
K3=KKZ(K)
RKX=AKR*DFLOAT(K1)
RKY=AKR*DFLOAT(K2)
RKZ=AKR*DFLOAT(K3)
RK2=AKR2*DFLOAT(K5)
KK=KS+1
N=NB(K)
CDK=DFLOAT(N)/6.DO
DO 101 M1=1,IA0BN0
IF(IA0BN0.EQ.IBOBN0) M2MAX=M1
DO 101 M2=1,M2MAX
IF(M1.NE.IA0BN0.OR.M2.NE.M2MAX) GO TO 101
ALP1=ALP(NORDA,M1)
ALP2=ALP(NORDB,M2)
W=1.DO/(ALP1+ALP2)
W4=W/4.DO
EXPA=RK2*W4
IF(DABS(EXPA).GT.EXPCVG) GO TO 101
ALAMDA=ALP1*ALP2*W
DELT=DSQRT(PI*W)
U1=ALP1*W
U2=ALP2*W
DSTP=U1*AHALF
MAXR=DSQRT(EXPCVG/ALAMDA)/AHALF+2.0
MR=DSQRT(FLOAT(ISQUNREND))!+1
IF(MAXR.GT.MR) MAXR=MR
CALL GSIFJFC(FCS1,RKX,NORD,NORDIM,NRDIM)
CALL GSIFJFC(FCS2,RKY,NORD,NORDIM,NRDIM)
CALL GSIFJFC(FCS3,RKZ,NORD,NORDIM,NRDIM)
DO 100 NRC=NRST,NREND
AX=AHALF*IX(NRC)
AY=AHALF*IY(NRC)
AZ=AHALF*IZ(NRC)
RAB2=AX*AX+AY*AY+AZ*AZ
EXPA=ALAMDA*RAB2
IF(EXPA.GT.EXPCVG) GO TO 101
RAB=DSQRT(RAB2)
AZETA=DEXP(-EXPA)
ADX=-U2*AX
ADY=-U2*AY
ADZ=-U2*AZ
HDX=U1*AX
BDY=U1*AY
BDZ=U1*AZ
CONST=AZETA*CN(NORDA,M1)*CN(NORDB,M2)*C0K
NRX=IX(NRC)+1
NRY=IY(NRC)+1
NRZ=IZ(NRC)+1
DO 111 I1=1,NORD
  S1=FCS1(I1,NRX)
  S2=FCS2(I1,NRX)
  S3=FCS3(I1,NRX)
DO 111 I2=1,NORD
  S4=FCS1(I2,NRY)
  S5=FCS2(I2,NRY)
  S6=FCS3(I2,NRY)
DO 111 I3=1,NORD
  IT=1+I2+I3-3
  IF(IT.GE.NORD) GO TO 111
  S7=FCS1(I3,NRZ)
  S8=FCS2(I3,NRZ)
  S9=FCS3(I3,NRZ)
  S=(S1*S3*S9+S4*S8*S3+S2*S6*S7+S3*S5*S7+S2*S4*S9+S1*S6*S8)*CONST
  IJ=((I1-1)*NORD+I2-1)*NORD+I3
  SIJ(IJ)=S
111 CONTINUE

C SUM OVER BINOMIAL EXPANSIONS IN FQ(2,43)
C IJAB=0,0
DO 201 IA3=1,NORDA
DO 201 IA2=1,NORDA
DO 201 IA1=1,NORDA
IA=IA1+IA2+IA3-2
IF(IA.TE.NORDA) GO TO 201
DO 202 IB3=1,NORDB
DO 202 IB2=1,NORDB
DO 202 IB1=1,NORDB
201 I J B = I J B + 1
202 CONTINUE
IF (IBT .NE. NORDB) GO TO 202

C1 = 1.0
DO 211 NA1 = 1, IA1
J A1 = IA1 - NA1 + 1
CA2 = CIJ (IA1, JA1)
DO 212 NA2 = 1, IA2
J A2 = IA2 - NA2 + 1
CA3 = CIJ (IA2, JA2)
DO 213 NA3 = 1, IA3
J A3 = IA3 - NA3 + 1
CB1 = CIJ (IA3, JA3)
DO 221 NB1 = 1, IB1
J B1 = IB1 - NB1 + 1
NAB1 = JA1 + JB1 - 1
CB2 = CIJ (IB1, JB1)
DO 222 NB2 = 1, IB2
J B2 = IB2 - NB2 + 1
NAB2 = JA2 + JB2 - 1
CB3 = CIJ (IB2, JB2)
DO 223 NB3 = 1, IB3
J B3 = IB3 - NB3 + 1
NAB3 = JA3 + JB3 - 1
CD = CIJ (IB3, JB3) * CA1 * CA2 * CA3 * CR1 * CB2 * CH3
NIJ = ((NAB1 - 1) * NORB + NAB2 - 1) * NORB * NAB3
T I J = TI J + CD * SJ (NI J)
CB3 = CB3 * BDZ
223 CONTINUE
CB2 = CB2 * BDY
222 CONTINUE
CB1 = CB1 * BDX
221 CONTINUE
CA3 = CA3 * ADZ
213 CONTINUE
CA2 = CA2 * ADY
212 CONTINUE
CA1 = CA1 * ADX
211 CONTINUE
IJAB = IJAB + 1
GI J = T I J
WRITE (1) NRC, M1, M2, IJAB, GI J
IF (K .EQ. 1) THEN
WRITE (6, 300) NRC, M1, M2, IJAB, IA1, IA2, IA3, IB1, IB2, IB3, T I J
202 CONTINUE
300 FORMAT (1X, 15, 3I4, 3X, 3I1, 1X, 3I1, 5X, F16.8)
201 CONTINUE
100 CONTINUE
101 CONTINUE
105 CONTINUE
    GO TO 999
1000 STOP
    END
PROGRAM 4. SUM OVER DIRECT LATTICE VECTORS FOR H, S, AND P MATRICES

**PERFORM THE SUM EXP(I K.R) H(R) OVER R**
**H IS STORED FOR INDEPENDENT R ONLY. THE GROUP OPERATIONS WHICH GENERATE**
**THE STAR OF R IS DONE IN THIS PROGRAM**

\[ A = \text{LATTICE CONSTANT} \]
\[ \alpha = \text{THE EXCHANGE PARAMETER} \]
\[ N_{\text{OBNO}} = \text{NO OF SYMMETRIES CONSIDERED =3 FOR S,P,AND D FUNCTIONS} \]
\[ \text{MAXA2} = \text{THE SQUARE OF THE MAXIMUM MAGNITUDE OF THE DIRECT LATTICE VECTORS} \]
\[ I_{\text{BZDIV}} = \text{DIVISION BETWEEN K=(0,0,0) AND K=(1,0,0)} \]
\[ L = \text{THE GROUP OPERATIONS WHICH GENERATE THE GROUP OPERATIONS WHICH GENERATE} \]
\[ \text{NCH0} = \text{GTO NUMBER} \]
\[ E = \text{S, P, D} \]
\[ N_{\text{ATOM}} = \text{ATOMIC BASIS NO.} \]
\[ N_{\text{ATOM}} = \text{C IF INDEPENDENT GTO ARE USED} \]
\[ N_{\text{ATOM}} = \text{NO OF DIRECT LATTICE VECTORS USED FOR S & P INTEGRALS} \]
\[ N_{\text{ATOM}} = \text{NO OF DIFFERENT TYPES OF MATRICES STORED} \]
\[ N_{\text{CHO(I)}} = \text{DETERMINES THE TYPE OF MATRICES TO BE CALCULATED} \]
\[ N_{\text{CHO(I)}} = \text{IF (NDIAG.NE.0.AND.NCHO(I).GT.NKIND) HAMILTONAIN IS DIAGONALIZED} \]
\[ IPRIT = \text{NO OF K POINTS TO BE PRINTED} \]
\[ N_{\text{CHO(I)}} = \text{THE WAVE VECTORS ARE ARRANGED IN THE FOLLOWING ORDER OF SYMMETRY} \]
\[ (X,Y,I), (I=1,LDMAX), (Z,I), (I=1,LDMAX), (ZX(I),I), (I=1,LDMAX), \]
\[ (Z2(I),I), (I=1,LDMAX), (S(I),I), (I=1,LSMAX), (PXi(I),I), (I=1,LPMAX) \]

**IMPLICIT REAL *8 (A-F,H-O-Z) REAL*4 SSA,SSB,PSA,PSB,SDA,SDB,PAA,PBB,PDA,PDB,DDA,DDB INTEGER *2 IX(100),YY(100),IZ(100),INB(100),KBX(89),KBY(89),KBZ(89)
INTEGER *2 NPUMPS(3,6),NPUMSD(6,6),NPUMP(9,6),NPUMPD(18,6),
& NPUMDD(36,6),NRTYS(3),NRTYP(9),NRTYD(18),NRTYDD(36)
& NDUM(3,3,3,3,3)
DIMENSION SICO(6,8),SINE(12,5),COSN(12,5),H(741),S(741),G(741)
DIMENSION X(38,38),G(741),G(38,38),GS(741)
DIMENSION DASGN(5,6),C(4,14),P(3,11),S(5,5),GIDEN(12)
DIMENSION ISQ(100)
DIMENSION ALS(14),ALP(11),ALD(5),COS(14),COP(14),COD(14)
DIMENSION GWTS(3)
COMMON/GTO/CRYSTL,PI,XATOM,IPATOM,IGATOM
COMMON/LCA/SSA(40,10),PSA(40,36),SDA(40,120),PAA(40,54),PDA(30,270)
& DDA(6,540)
COMMON/LCB/SSR(1,1),PSB(1,1),SBR(1,1),PBB(1,1),PDB(1,1),DDB(1,1)
COMMON/LCB/SSR(40,10),PSB(40,36),SBR(40,120),PBB(40,54),PDB(30,270)
& DDB(6,540)
COMMON/OBNO/ALPHA,NKIND,NTOL,NCOD(5),NSYM
DATA GIDEN/'COUL','EXCH','EXUP','EXDN','KINE','OVLP','PX','PY','
& PZ','HPA','HP U','HDN'/'
DATA GWSPD/*^*P*,*D*/
1 FORMAT(A8,F12.5,F10.8,10I5)
READ(5,1) CRYSTL,A,ALPHA,ICUB,MXBNO,MAXA2,IA DIM,IBZDIV,NDIM
PI=3.1415926535897932
AKRBZ=2.DO*PI/(A*DFLOAT(18ZDIV))
K3ZPT=IBZD I  V ♦ 1
AHALF=A/2.DO
IF (IDCUB.EQ.1) AHALF=A
OMEGA=A**3/DFLOAT(IDCUB)
4 FORMAT(1615)
READ(5,4) IASS, IAPS, IASD, IAPP, IADO
READ(5,4) NKIND, NTOL, (NCHO(J), J=1,NTOL)
WRITE(6,3) ALPHA, NKIND, (GIDEN(NCHO(I)), I=1,NTOL)
3 FORMAT(/,1X,'EXCH PARAMETER=',F10.6,10X,'NO READ=',5S,5X,(3X,A4))
NSYMP=0
IF (NCHO(1).GT.NKIND-3.AND.,NCHO(1).LT.NKIND) NSYMP=1
READ IN THE EXPANSION COEFFICIENTS IN THE ATOMIC BASIS FUNCTIONS
READ(5,4) ISOBNO, ISATOM, IPOBNO, IPATOM, IDOBNO, IDATOM
LSMAX=ISOBNO
LDMAX=IDOBNO
LPMAX=IPOBNO
IF (ISATOM.NE.0) LSMAX=ISATOM
IF (IDATOM.NE.0) LDMAX=IDATOM
IF (IPATOM.NE.0) LPMAX=IPATOM
CALL RDGTO(ALS,ALP,ALD,ALS,ALD,ALD,ISOBND,LSMAX,IPOBNO,
LPMAX,ISOBNO,LDMAX,0)
ISSDIM=LSMAX*(LSMAX+1)/2
IPDDIM=9*LPMAX*(LPMAX+1)/2
IPDDIM=36*LDMAX*(LDMAX+1)/2
IPDDIM=6*LSMAX*LDMAX
IPDDIM=18*LPMAX*LDMAX
LDST=1
LOEND=LDMAX*5
LSST=LOEND+1
LSEND=LOEND+LSMAX
LPST=LSSEND+1
LPEND=LSEND+LPMAX*3
NB=LPEND
NBTRI=NB*(NB+1)/2
WRITE(6,5) IASS, ISSDIM, IAPS, IPDDIM, IASD, ISSDIM, IAPP, IPDDIM,
IAPD, IPDDIM, IADD, IPDDIM
5 FORMAT(/,1X,'SS=(',12I5,'),2X,'PS=(',12I5,')',2X,'SD=(',12I5,')',2X,'PP=(',12I5,')',2X,'PD=(',12I5,')',2X,'DD=(',12I5,')')
IDC = 1
IF(IDCUB .NE. 1) IDC = 8 / IDCUB

GENERATE INDEPENDENT DIRECT LATTICE VECTORS
CALL GINDPK(I X, I Y, I Z, ISQU, I ADIM, IDC, MAXA2, INB, 1, 1)

5310 FORMAT(6I5)
DO 60 I = 1, I ADIM
WRITE(6, 5310) I, IX(I), IY(I), IZ(I), INB(I)
60 CONTINUE

GENERATE EQUALLY SPACED POINTS IN THE 1/48TH OF THE INDEPENDENT B.Z.
CALL GBZPT(KBX, KBY, KBZ, WT, NKPT, IDCUB, KBZPT, SUMW)
WRITE(6, 2) CRYSTL, A, IDCUB, MXOBNO, MAXA2, I ADIM, NKPT, NRDIM, KBZPT,
1 GWTSFD(1), ISOBNO, ISATOM, GWTSFD(2), IPOBNO, IPATOM, GWTSFD(3), IDOBNO,
2 IATOM
2 FORMAT(1X, A8, 2X, 'LATTICE CONST=', F10.5, 3X, 'ATOMS/LATTICE=', I5, 3X,
1 MAX N=', I5, 3X, 'MAX A2=', I5, 3X, 'A DIM=', I4, 3X, 'NKPT=', I5, 3X,
2 'DIMENSION SINE(*215, *)', 3X, '/1X, 3(A2, 3 'ORBITAL NO=', I4, 2X, 'ATOMIC NO=', I4, 2X, ')

DEFINE THE EXPANSION COEFFICIENTS FOR THE D FUNCTION WITH CUBIC SYMERY

DO 90 I = 1, 5
DO 90 J = 1, 6
90 DASIGN(I, J) = 0.00
DASIGN(1, 2) = 1.00
DASIGN(2, 5) = 1.00
DASIGN(3, 4) = 1.00
DASIGN(4, 1) = 0.50
DASIGN(4, 3) = -0.500
C3 = 0.500 / DSQRT(3.00)
DASIGN(5, 1) = -C3
DASIGN(5, 3) = -C3
DASIGN(5, 6) = 2.00 * C3
MAXR = SQRT(FLOAT(MAXA2)) + 2
RD = 0.00
DO 70 NR = 1, MAXR
RKZ = 0.00
DO 71 KB = 1, KBZPT
RK = RD * RKZ
SINE(NR, KB) = DSIN(RK)
COSN(NR, KB) = DCOS(RK)
71 RKZ = RKZ + AKRBZ
RD = RD + AHALF
DEFINE THE GROUP OPERATIONS THAT GENERATE THE STAR OF R
FINDS THE TERM IN THE EXPANSION OF \( \exp(I K \cdot R) \) WHICH IS AN EVEN
FUNCTION OF RX, RY, AND RZ.

CALL GNOPUM(NPUMPS,NTYPS,NDUM,MXORNO,3,2,1,NSYMP)
CALL GNOPUM(NPUMSD,NTYSD,NDUM,MXORNO,6,1,3,NSYMP)
CALL GNOPUM(NPUMPP,NTYPP,NDUM,MXORNO,9,2,2,NSYMP)
CALL GNOPUM(NPUMPD,NTYPD,NDUM,MXORNO,18,2,3,NSYMP)
CALL GNOPUM(NPUMDD,NTYDD,NDUM,MXORNO,36,3,3,NSYMP)

SUBROUTINE READ (READ) READS IN THE INTEGRALS GENERATED IN PROGRAM 2 OR 3

CALL READ(SSA,PSA,SDA,PPA,PDA,DDA,SSB,PSB,SOB,PPR,DDR,ODR,DSR,  
1IAS, 1APS, 1ASD, 1APP, 1ADD, 1ISSDIM, 1IPSDIM, 1ISDDIM, 1IPDDIM,  
2IPDDIM, 1IODDIM, CS, CP, CD, LSSMAX, ISOBNO, LPMAX, IPDBNO, LDMAX, IDORN0)

READ(5,4,END=10000) KPTST,KPTFND,NDIAG,IPRINT,IPUNCH

PRINT 915
DO 1000 KPT=KPTST,KPTEND
DO 80 1=1,NBTRI
H(1)=0.DO
S(1)=0.DO
KX=KBX(KPT)
KY=KBY(KPT)
KZ=KBZ(KPT)
K1=KX+1
K2=KY+1
K3=KZ+1
DO 900 NRC=1,IADIM
I1=I(X(NRC))+1
I2=IY(NRC)+1
I3=IZ(NRC)+1
CALL GSICO(SICO,SINF,COSN,NRDIM,KBZPT,K1,K2,K3,I1,I2,I3)
N=INB(NRC)
CONST=OFLOAT(N)/6.DO

SS=S

IF(NRC.GT.IASS) GO TO 150
SCSS=(SICO(1,1)+SICO(2,1)+SICO(3,1)+SICO(4,1)+SICO(5,1)+SICO(6,1))

*CONST
M1=0
DO 100 M1=LSTT,LSSEND
DO 100 M2=LSST,M1
M1=M1+1
\[
    IJ = M_1 \times (M_1 - 1) / 2 + M_2 \\
    H(IJ) = H(IJ) + SSA(NRC, M_1) \times SCSS \\
    IF(NTOL, GT, 1) S(IJ) = S(IJ) + SSB(NRC, M_1) \times SCSS \\
    100 \ CONTINUE \\
    150 \ CONTINUE \\
    \\
    P = S \\
    IF(NRC, GT, IAPS) GO TO 250 \\
    M_1 = 0 \\
    DO 200 M_1 = 1, LPMAX \\
    IP = (M_1 - 1) + 3 \times LSEND \\
    DO 200 M_2 = LSST, LSEND \\
    M_1 = M_1 + 1 \\
    IL = (M_1 - 1) \times 3 \\
    DO 210 NM = 1, 3 \\
    MP = IP + NM \\
    IJ = MP \times (MP - 1) / 2 + M_2 \\
    NT = NTYPS(NM) \\
    DO 211 L = 1, 6 \\
    NL = IL + NPUMPS(NM, L) \\
    H(IJ) = H(IJ) + PS(A(NRC, NL) \times SICO(L, NT) \times CONST \\
    IF(NTOL, GT, 1) S(IJ) = S(IJ) + PSB(NRC, NL) \times SICO(L, NT) \times CONST \\
    211 \ CONTINUE \\
    210 \ CONTINUE \\
    200 \ CONTINUE \\
    250 \ CONTINUE \\
    \\
    S = D \\
    IF(NRC, GT, IASD) GO TO 350 \\
    M_1 = 0 \\
    DO 300 M_1 = LSST, LSEND \\
    DO 300 M_2 = 1, LDMAX \\
    II = M_1 \times (M_1 - 1) / 2 + M_2 \\
    M_1 = M_1 + 1 \\
    IL = (M_1 - 1) \times 6 \\
    DO 310 NM = 1, 6 \\
    NT = NTYSD(NM) \\
    CA = 0.00 \\
    CB = 0.00 \\
    DO 311 L = 1, 6 \\
    NL = IL + NPUUSSD(NM, L) \\
    CA = CA + SDA(NRC, NL) \times SICO(L, NT) \times CONST \\
    IF(NTOL, GT, 1) CB = CB + SDB(NRC, NL) \times SICO(L, NT) \times CONST \\
    311 \ CONTINUE
DO 312 I=1,5
   IJ=I+(I-1)*LDMAX
   H(IJ)=H(IJ)+CA*DA5IGN(I,NM)
   CONTINUE
312 CONTINUE
310 CONTINUE
300 CONTINUE
350 CONTINUE

C C
IF(NRC.GT.IAPP) GO TO 450
MI=0
DO 400 M1=1,LPMAX
   IP1=(M1-1)*3+LSEND
   DO 400 M2=1,M1
      IP2=(M2-1)*3+LSFND
      IF(MI.TE.GT.MTOL*GT.1) S(IJ)=S(IJ)+CB*DA5IGN(I,NM)
      CONTINUE
   CONTINUE
400 CONTINUE
450 CONTINUE

C C
IF(NRC.GT.IAPP) GO TO 550
MI=0
DO 500 M1=1,LPMAX
   IP=(M1-1)*3+LSEND
   DO 500 M2=1,LDMAX
      MI=MI+1
      IL=(MI-1)*9
      NM=0
      DO 410 N1=1,3
         MP1=IP1+N1
         DO 410 N2=1,3
            MP2=IP2+N2
            NM=NM+1
            IF(MP1.LT.MP2) GO TO 410
            IJ=MP1*(MP1-1)/2+MP2
            NT=NTYPP(NM)
            DO 411 L=1,6
               NL=IL+NPUMPP(NM,L)
               H(IJ)=H(IJ)+PPA(NRC,NL)*SICO(L,NT)*CONST
               IF(NTOL.GT.1) S(IJ)=S(IJ)+PPB(NRC,NL)*SICO(L,NT)*CONST
            CONTINUE
   CONTINUE
410 CONTINUE
411 CONTINUE
500 CONTINUE
550 CONTINUE

C C
IF(NRC.GT.IAPPD) GO TO 550
MI=0
DO 500 M1=1,LPMAX
   IP=(M1-1)*3+LSEND
   DO 500 M2=1,LDMAX
      MI=MI+1
      IL=(MI-1)*18
      CONTINUE
500 CONTINUE
550 CONTINUE
NM = 0
DO 510 NI = 1, 3
NP = NP + 1
II = NP * (NP - 1) / 2 + 1
DO 510 N2 = 1, 6
NM = NM + 1
NT = NYPD(NM)
CA = 0.0
CB = 0.0
DO 511 L = 1, 6
NL = IL + NYPD(NM, L)
CA = CA + PDA(NRC, NL) * SICO(L, NT) * CONST
IF (NTOL. GT. 1) CB = CB + PDB(NRC, NL) * SICO(L, NT) * CONST
511 CONTINUE
DO 512 I = 1, 5
IJ = I + (I - 1) * LDMAX
H(IJ) = H(IJ) + CA * DASIGN(I, N2)
IF (NTOL. GT. 1) S(IJ) = S(IJ) + CB * DASIGN(I, N2)
512 CONTINUE
510 CONTINUE
500 CONTINUE
550 CONTINUE
D - D
IF (NRC. GT. LADD) GO TO 650
DO 600 M1 = 1, LDMAX
DO 600 M2 = 1, LDMAX
IF (M1. GE. M2) M1 = M1 * (M1 - 1) / 2 + M2
IF (M1. LT. M2) M1 = M2 * (M2 - 1) / 2 + M1
IL = (M1 - 1) * 36
DO 610 N1 = 1, 6
DO 610 N2 = 1, 6
IF (M1. GE. M2) NM = (N1 - 1) * 6 + N2
IF (M1. LT. M2) NM = (N2 - 1) * 6 + N1
NT = NYDD(NM)
CA = 0.0
CB = 0.0
DO 611 L = 1, 6
NL = IL + NYPD(NM, L)
CA = CA + PDA(NRC, NL) * SICO(L, NT) * CONST
IF (NTOL. GT. 1) CB = CB + PDB(NRC, NL) * SICO(L, NT) * CONST
611 CONTINUE
613 CONTINUE
DO 612 I = 1, 5
ND1 = M1 * (I - 1) * LDMAX
DO 612 I2=1,5
ND2=M2*(I2-1)*LDMA
IF(ND1.LT.ND2) GO TO 612
IJ=ND1*(ND1-1)/2+ND2
H(IJ)=H(IJ)+CA*DASIGN(I1,N1)*DASIGN(I2,N2)
IF(NTOL.GT.1) S(IJ)=S(IJ)+CB*DASIGN(I1,N1)*DASIGN(I2,N2)
612 CONTINUE
610 CONTINUE
600 CONTINUE
650 CONTINUE
900 CONTINUE
GT=T(KPT)
820 FORMAT(20X,'i5,t15('i4,t15'x')i4,t15'x'),5X,')
WRITE(6,820) KPT,KX,KY,KZ,GT
NOPT=0
810 CONTINUE
NOPT=NOPT+1
DO 850 I=1,NBTR1
IF(NTOL.GT.1) GS(I)=S(I)
850 CONTINUE
WRITE(2) KX,KY,KZ,GT,GF
IF(NTOL.GT.1) WRITE(3) KX,KY,KZ,GT,GS
IJ=0
DO 800 I=1,NB
DO 800 J=1,I
IJ=IJ+1
IF(NOPT.EQ.2) GO TO 801
X(I,J)=H(IJ)
X(J,I)=H(IJ)
801 CONTINUE
X(I,J)=S(IJ)
X(J,I)=S(IJ)
800 CONTINUE
IF(NDIAG.EQ.0) GO TO 1001
IF(NCHD(NOPT).LE.NK1ND) GO TO 1002
C CALCULATE THE ENERGY EIGENVALUES (GE) AND EIGENVECTORS (GX)
C THE OVERLAP MATRIX (S) IS EXPRESSED AS THE PRODUCT OF A UPPER TRIANGULAR
C MATRIX (R) AND ITS TRANSPOSE (R**T)
C H* X = X' E , WHERE H*=(R**T)**-1) H (R**-1) AND X'= R X
C SUBROUTINES DMDS AND DMFSD ARE IN IBM SCIENTIFIC SUBROUTINE PACKAGE.
C DIGEN IS THE DOUBLE PRECISION VERSION OF SUBROUTINE EIGEN IN IBM S.S.P.
A = 10.**(-9)
CALL DMFSD(S,M,A,IE1)
CALL DMTDS(X,NB,NB,S,-1,IF2)
CALL DMTDS(X,NB,NB,S,2,IF3)
DO 7150 I=1,NB
    DO 7150 J=1,I
        IJ=I*(I-1)/2+J
    7150 H(IJ)=X(I,J)
        CALL OIGEN(H,X,NB,0)
        CALL DMTDS(X,NB,NB,S,1,IF4)
        CALL OIGEN(H,X,NB,0)
        CALL DMTDS(X,NB,NB,S,1,IF4)
        CALL OIGEN(H,X,NB,0)
        CALL DMTDS(X,NB,NB,S,1,IF4)
        IF (IF1.NE.0.OR(IF2.NE.0.OR(IF3.NE.0.OR(IF4.NE.0))) WRITE(6,844) IE1,
            IE2,IE3,IE4
        DO 3561 I=1,NB
            IJ=I*(I-1)/2+I
            GF(I)=H(IJ)
        3561 DO 3561 J=1,NB
            GX(I,J)=X(I,J)
        3561 DO 3561 J=1,NB

344 FORMAT(1H0,1X,IER=.,4F15)
IF (IF1.NE.0.OR.IF2.NE.0.OR.IF3.NE.0.OR.IF4.NE.0) WRITE(6,844) IE1,
    IE2,IE3,IE4
444 FORMAT(1H0,1X,IER=.,4F15)
444 FORMAT(1H0,1X,IER=.,4F15)
444 FORMAT(1H0,1X,IER=.,4F15)
444 FORMAT(1H0,1X,IER=.,4F15)
444 FORMAT(1H0,1X,IER=.,4F15)
444 FORMAT(1H0,1X,IER=.,4F15)
444 FORMAT(1H0,1X,IER=.,4F15)
444 FORMAT(1H0,1X,IER=.,4F15)
444 FORMAT(1H0,1X,IER=.,4F15)
444 FORMAT(1H0,1X,IER=.,4F15)
444 FORMAT(1H0,1X,IER=.,4F15)
444 FORMAT(1H0,1X,IER=.,4F15)
444 FORMAT(1H0,1X,IER=.,4F15)
444 FORMAT(1H0,1X,IER=.,4F15)
444 FORMAT(1H0,1X,IER=.,4F15)
444 FORMAT(1H0,1X,IER=.,4F15)
444 FORMAT(1H0,1X,IER=.,4F15)
444 FORMAT(1H0,1X,IER=.,4F15)
444 FORMAT(1H0,1X,IER=.,4F15)
444 FORMAT(1H0,1X,IER=.,4F15)
444 FORMAT(1H0,1X,IER=.,4F15)
444 FORMAT(1H0,1X,IER=.,4F15)
444 FORMAT(1H0,1X,IER=.,4F15)
444 FORMAT(1H0,1X,IER=.,4F15)
444 FORMAT(1H0,1X,IER=.,4F15)
444 FORMAT(1H0,1X,IER=.,4F15)
444 FORMAT(1H0,1X,IER=.,4F15)
PRINT 811
DO 913 I=1,NB
  913 WRITE(6,914) (X(I,J),J=I1,I2)
  PRINT 915
    IF(12.LT.NB) GO TO 912
    IF(NOPT.LE.NTOL.AND.NDIAG.EQ.C) GO TO 910
    914 FORMAT(1X,10F13.5)
    915 FORMAT(1H1)
1000 CONTINUE
    GO TO 999
10000 CONTINUE
STOP
END
PROGRAM 5. BLOCH BASIS FUNCTION ALONG THREE PRINCIPLE DIRECTIONS.

ACONST=LATTICE CONSTANT (IN A. U.)
EXPCVG=CONVERGENT CRITERIAL. EXP(-EXPCVG)=0.0
IDCUB=NUMBER OF ATOMS PER LATTICE
MAXA2=THE SQUARE OF THE MAXIMUM MAGNITUDE OF THE DIRECT LATTICE VECTORS
DIMENSION IA(IADIM) ECT.
IBZDIV=DIVISION BETWEEN K=(0,0,0) AND K=(1,0,0)*2*PI/A
ISOBNO=GTO NUMBER. &S, P, D
ISATOM=ATOMIC BASIS NO. ISATOM=0 IF INDEPENDENT GTO ARE USED
NPGAUS=NO OF POINTS USED IN THE GAUSSIAN INTEGRATION OVER THE WIGNER-SEITZ
SPHERE (CALCULATING THE FOURIER COEFFICIENTS OF THE EXCHANGE POTENTIAL)

IMPILCIT REAL *8 (A-F,H,O-Z)
COMPLEX*8 BASF(38),SC,COSC
COMPLEX*8 GRASF(38)
INTEGER*2 IAX(500),IAY(500),IAZ(500),ISQU(500)
INTEGER*2 KBX(89),KBY(89),KBZ(89)
DIMENSION WT(89)
DIMENSION R(96),W(96),Y(100)
DIMENSION AX(500),AY(500),AZ(500),PRMX(48),PRMY(48),PRMZ(48)
DIMENSION ALS(14),ALP(11),ALD(5),COS(14),COP(11),COD(5),CS(4,14),
&C(3,11),CD(5,5)
COMMON/GTO/CRYSTL,PI,ISATOM,IPATOM,IDATOM
PI=3.141592653589793
51 FORMAT(2X,A8,2F10.5,10I5)
READ(5,51) CRYSTL,ACONST,EXPCVG,IDCUB,IBZDIV,IADIM,MIXA2,NPGAUS
OMEGA=ACONST**3/DFLOAT(IDCUB)
DIV=DFLOAT(IBZDIV)
*GSZRO=(0.75D0*OMEGA/PI)**0.3333333D0

DEFINE GAUSSIAN EXPONENTS AND EXPANSION COEFFICIENTS
4 FORMAT(815)
READ(5,4) ISOBNO,ISATOM,IPOBNO,IPATOM,IDOBNO,IDATOM
LSMAX=ISOBNO
LDMAX=IDOBNO
LPMAX=IPOBNO
IF(ISATOM.NE.0) LSMAX=ISATOM
IF(IDATOM.NE.0) LDMAX=IDATOM
IF(IPATOM.NE.0) LPMAX=IPATOM
CALL ROGTO(ALS,ALP,ALD,COS,COP,COD,CS,CP,CD,ISOBNO,LSMAX,IPOBNO,
&LPMAX,IDOBNO,LDMAX,1)
LST=1
LDEND=LDMAX*5
LSST=LDEND+1
LSEND=LDEND+LMAX
LPST=LSEND+1
LPEND=LSEND+LMAX*3
PRINT 59
59 FORMAT(1H1)

GENERATE EQUALLY SPACED POINTS IN THE 1/48TH OF THE INDEPENDENT R, Z.

IBZPT=IBZDIV+1
CALL GBOZPT(KBX,KRY,KBZ,WT,NKPT,IDCUB,IBZPT,SWM)
IDC=8/IDCUB
IF(IDCUB.EQ.1) IDC=1
CALL GPERMK(IAX,IAY,IAZ,ISQU,IADIM,IDC,MAXA2,1)
IF(IDCUB.EQ.1) AHALF=ACONST
IF(IDCUB.EQ.1) AHALF=ACONST/2.0D
DO 70 I=1,IADIM
   AX(I)=AHALF*IAX(I)
   AY(I)=AHALF*IAY(I)
   AZ(I)=AHALF*IAZ(I)
70 CONTINUE
WRITE(6,52) ACONST,IDCUB,IBZDIV,IADIM,MAXA2,NPGAUS,LMAX,
& ISOBNO,LPMAX,IPOBNO,LDMAX,IDORNO,EXPVG
52 FORMAT(1X,'LATTICE CONST= ',F10.5,2X,'ATOMS/LATTICE= ',
   1I5,2X,'B,Z, DIV= ',I5,2X,' R NO= ',I7,2X,' MAX R**2= ',I5,
   22X,'GAUS NO= ',I5,2X,'1 X,5= (',I5,2I5,')',2X,'P= (',I5,2I5,')',2X,'D= (',I5,
   3,')',5X,'EXP MAX= ',F10.2,/) C

DEFINE R AND WEIGHT FACTOR FOR GAUSSIAN INTEGRATION OVER THE WIGNER-SFITZ SPHERE

CALL GWTGAS(NPGAUS,Y,R,W)
DO 54 I=1,NPGAUS
54 R(I)=WGSZRO*(R(I)+1.0D)/2.0D

READ IN PERMUTED VECTORS ALONG THREE PRINCIPLE DIRECTIONS
NPTOL=PERMUTATION NUMBER FOR EACH DIRECTION

90 FORMAT(3F10.4)
I=0
91 READ(5,4,END=999) NPTOL
DO 92 J=1,NPTOL
   I=I+1
   READ(5,90) PRMX(I),PRMY(I),PRMZ(I)
   RNORM=DSQRT(PRMX(I)**2+PRMY(I)**2+PRMZ(I)**2)
   PRMX(I)=PRMX(I)/RNORM
92 CONTINUE
PRMY(I) = PRMY(I)/RNORM
PRMZ(I) = PRMZ(I)/RNORM

CONTINUE
GO TO 91

CONTINUE
ITOL = I

FORMAT(15, 3F10.1)
CK = 2.0D0*PI/ACONST/DIV
DO 100 KPT = 1, NKPT
    RKX = CK*KBX(KPT)
    RKY = CK*KBY(KPT)
    RKZ = CK*KBZ(KPT)
    DO 200 I0 = 1, NPGAUS
    DO 300 NPNO = 1, ITOL
        RX = R(I0)*PRMX(NPNO)
        RY = R(I0)*PRMY(NPNO)
        RZ = R(I0)*PRMZ(NPNO)
        DO 510 I = 1, LPEND

CONTINUE

CONTINUE

BASF(I) = (0.0D0, 0.0D0)

SUM OVER PERMUTED DIRECT LATTICE VECTORS

DO 500 NRC = 1, NRTOL
    PX = RX+AX(NRC)
    PY = RY+AY(NRC)
    PZ = RZ+AZ(NRC)
    PP = PX*PX+PY*PY+PZ*PZ
    RK = RKX*AX(NRC)+RKY*AY(NRC)+RKZ*AZ(NRC)
    SINE = DSIN(RK)
    COSINE = DCOOS(RK)
    SC = DCMPLX(COSINE, SINE)

S-WAVE FUNCTIONS

DO 520 NS = 1, ISOBNO
    DEL = PP*ALS(NS)
    IF(DEL.GT.EXPCVG) GO TO 520
    CONST = DEXP(-DEL)
    DO 21 IS = 1, LMAX
        I1 = IS+L Max
        CO = CONST*CS(IS, NS)
        BASF(I1) = BASF(I1) + SC*CO
    21 CONTINUE

CONTINUE

P-WAVE FUNCTIONS


C
DO 530 NP=1,IPDBNO
DEL=PP*ALP(NP)
IF(DEL.GT.EXPCVG) GO TO 530
CONST=EXP(-DEL)
DO 31 IP=1,LMAX
II=3*(IP-1)
IX=II+LSEND+1
IY=II+LSEND+2
IZ=II+LSEND+3
CONST=EXP(-DEL)
DO 31 IP=1,LMAX
IX=II+LSEND+1
IY=II+LSEND+2
IZ=II+LSEND+3
CO=CONST*CP(IP,NP)
COSC=CO*SC*(0.00,-1.00)
BASF(IX)=BASF(IX)+COSC*PX
BASF(IY)=BASF(IY)+COSC*PY
BASF(IZ)=BASF(IZ)+COSC*PZ
31 CONTINUE
530 CONTINUE
C
D-WAVE FUNCTIONS
C
PXY=PX*PY
PYZ=PY*PZ
PZX=PZ*PX
PZ2=(PZ*PZ-PY*PY)/2.DO
PZ2=(3.DO*PZ*PZ-PP)/(2.DO*DSQRT(3.DO))
DO 540 ND=1,IPDBNO
DEL=PP*ALD(ND)
IF(DEL.GT.EXPCVG) GO TO 540
CONST=EXP(-DEL)
DO 41 ID=1,LMAX
NDXY=ID
NDYZ=NDXY+LMAX
NDXZ=NDYZ+LMAX
NDX2=NDXZ+LMAX
NDZ2=NDX2+LMAX
CO=CONST*CD(ID,ND)
COSC=SC*CO
BASF(NDXY)=BASF(NDXY)+COSC*PXY
BASF(NDYZ)=BASF(NDYZ)+COSC*PYZ
BASF(NDXZ)=BASF(NDXZ)+COSC*PZX
BASF(NDX2)=BASF(NDX2)+COSC*PX2
BASF(NDZ2)=BASF(NDZ2)+COSC*PZ2
41 CONTINUE
540 CONTINUE
500 CONTINUE
DO 700 I=1,LPEND
700  GBASF(I) = BASF(I)
      WRITE(1) GBASF
300  CONTINUE
      WRITE(6,750) RX,RY,RZ,(BASF(I),I=1,LPEND)
      PRINT 751
750  FORMAT(9E14.6)
751  FORMAT(1H0)
200  CONTINUE
100  CONTINUE
400  CONTINUE
1090 CONTINUE
STOP
END
PROGRAM 6. SELF-CONSISTENCY

************

ACINST=LATTICE CONSTANT (IN A. U.)
ALPHA=THE EXCHANGE PARAMETER
FACT=PARAMETER USED TO SPEED UP THE SELF-CONSISTENT PROCEDURE
ELECT=NUMBER OF ELECTRONS PER ATOM
DEN=ENERGY GRID SIZE USED IN CALCULATING THE DENSITY OF STATES.
IDCUB=NUMBER OF ATOMS PER LATTICE
KNMAX=NO. OF RECIPROCAL LATTICE VECTORS CONSIDERED.
NEN=NO. OF POINTS USED IN CALCULATING THE DENSITY OF STATES
IBZDIV=DIVISION BETWEEN $K=(0,0,0)$ AND $K=(1,0,0)*2*PI/A$
NB=NO. OF BASIS FUNCTIONS.
NPGAUS=NO. OF POINTS USED IN THE NUMERICAL GAUSSIAN INTEGRATION OVER 
THE WIGNER-SEITZ SPHERE. (THE EXCHANGE POTENTIAL)

IF(IPUN.NE.0) PUNCH THE CHARGE DENSITY AND THEIR FOURIER COEFFICIENTS

************

REAL*8 XUP,XDN,X1,X2,T,OV,HUP,HDN,TN,QN,AA,BB,CC,S,W,AC,DD,WT

INTEGER*2 KX(89),KY(89),KZ(89),IX(51),IY(51),IZ(51),NN

DIMENSION W(96),R(96),DUP(96),DDN(96),DENUP(96),DENDN(96),RK(51)

DIMENSION S1J(741)

DIMENSION COUP(288),COND(288),VAUP(288),VADN(288)

DIMENSION VUPR(96),VDRN(96),VSMUP(51),VSDN(51)

DIMENSION XUP(38),XDN(38),X1(38,38),X2(38,38),T(741),OV(741),

2 VMUP(51),VMDN(51),DKUP(51),DKDN(51),EXUP(51),S(741),

3 VXDN(51),DK(51),VK(51),VXUP(51),VXDN(51),KK(51),VK(51),CON(51),

4 VXUP(51),VXDN(51),CKUP(51),CKDN(51),VKUP(51),VKDN(51)

DIMENSION WTDIR(3),NPUM(3)

DIMENSION HUP(38,38),HDN(38,38)

COMMON/LCS/TSW(3000),EN(3000),SW(3000)

COMMON/LCS/HUP,HDN,T,S

COMMON WT(89)

DATA NPUM/6,12,8/,WTDIR/C.28571419,0.45714266,0.25714275/

PI=3.141592653589793

1 FORMAT(6F12.8)

READ(5,1) ACONST,ALPHA,FACT,ELECT,DEN

READ(5,2) IDCUB,KNMAX,NEN,IBZDIV,NB,NPGAUS,IPUN

2 FORMAT(2015)

OMEGA=ACONST**3/DFLOAT(IDCUB)

KBZPT=IBZDIV+1

AKR=2.0D0*PI/ACONST

AKR2=AKR*AKR

ONETHD=1.0D0/3.0D0

SIXPI=-6.0D0*(3.0D0/4.0D0/PI)**.33333333
$$R_0 = (3.0 \times \Omega \times 4.0 / \pi)^{0.3333333}$$

$$C_{00} = -16.0 \times \pi \times \pi / (3.00 \times \Omega)$$

$$NBST = NB - 14$$

$$NBEND = NB - 9$$

$$NCST = NBEND + 1$$

DO 383 IRLV = 1, KNMAX

$V_K( IRLV ) = 0.0$

$V_{XUP}( IRLV ) = 0.0$

$383 \ V_{XDON}( IRLV ) = 0.0$

READ THE FOURIER COEFFICIENTS OF THE COULOMB AND EXCHANGE POTENTIALS AND THE CHARGE DENSITY. (OUT PUT OF PROGRAM 1)

DO 3712 J = 1, KNMAX

READ(8) KS, VKO(J), VX, VXUP(J), VXODN(J), VMUP(J), VMDN(J), IX(J), IY(J)

ORIZ(J), NN

CON(J) = NN

$AA = AKR2 \times FLOAT(KS)$

$RK(J) = DSORT(AA)$

$RKK(J) = -AA / 8.0 / \pi$

$VMSUP(J) = VMUP(J)$

$VMSDN(J) = VMDN(J)$

3712 CONTINUE

READ THE INITIAL CHARGE DENSITY CALCULATED IN PROGRAM 1.

DO 41111 I = 1, NPGAUS

41111 READ(5, 4089) R(I), W(I), DUP(I), DDN(I)

4089 FORMAT(4E14.8)

GENERATE EQUALLY SPACED POINTS AND THE CORRESPONDING WEIGHT FACTORS IN 1/48TH OF THE INDEPENDENT BRILLIOUN ZONE

CALL GBZPT(KK, KY, KZ, KT, NKPT, IDUB, KBZPT, SUMW)

WRITE(6, 3) ACONST, ALPHA, FACT, ELECT, DEN, NKPT, KNMAX, IDUB, NEN

& IBZDIV, NB, NPGAUS

3 FORMAT(1X, 'LATTICE CONST=', F10.5, 2X, 'EXCH PARA=', F10.5, 2X,


2**DE=', F10.5, 2X, 'NO=', F8.2, 'ATOMS/LATTICE=', F15.2, 'DE NO=', F15.2,

3**B.Z. DIV=', F15.2, 'BAND NO=', F15.2, 'GAUS NO=', F15.2, ')

1206 FORMAT(3I5)

PERFORM ITERATION NUMBER ITEROD+1 TO ITFRNW.

IF(NPART .NE. 0) THE FIRST HALF OF THE CALCULATION HAS BEEN DONE.

READ(5, 1206) ITEROD, ITFRNW, NPART
IF(NPART .NE. 0) READ(5, 1207) FERMIE
1207 FORMAT(F12.8)
IF(ITEROD .EQ. 0) GO TO 23510

C READ THE CORRECTIONS DUE TO SELF-CONSISTANCY IN THE PREVIOUS ITERATIONS.
C
DO 35610 ITER=1, ITEROD
35610 CONTINUE
ITERST=ITEROD+1
DO 32323 ITER=ITERST, ITERNEW
IF(NPART .NE. 0 .AND. ITER .LE. ITERST) GO TO 381
DO 2011 I=1, NEN
SW(I)=0.0
2011 CONTINUE
DO 12000 NM=1, NKPT
WRITE(6, 222) KX(NM), KY(NM), KZ(NM), NM, WT(NM)
222 FORMAT(3HK=I, 3AI, 1H 1, 5X, *NM = •  ♦  15.5X, •  W T  = *  .F 8.5, /)
9905 FORMAT(5A4)

C READ THE ORIGINAL COULOMB, KINETIC, EXCHANGE, AND OVERLAP MATRICES.
C
DO 370 I=1, NB
DO 370 J=1, I
IJ=J+([I-I]/2
READ(4, 9905) PO, EK, UP, DN, OVLP
HUP(I, J)=PO*EK+UP*ALPHA
HDN(I, J)=PO*EK+DN*ALPHA
OV(IJ)=OVLP
370 CONTINUE
Q FORMAT(A4)
DO 300 IRLV=1, KNMAX

C CALCULATE THE HAMILTONIAN OBTAINED FROM LAST ITERATION BY THE GENERALIZED
C OVERLAP MATRICES.
C
READ(I) SIJ
AA=VK(I)+VXUP( IRLV )*ALPHA
BB=VK(I)+VXDN( IRLV )*ALPHA
DO 300 I=1, NB
DO 300 J=1, I
IJ=I*(I-I)/2+J
HUP(I, J)=HUP(I, J)+AA*SIJ(IJ)
HDN(I, J)=HDN(I, J)+BB*SIJ(IJ)
HUP(J, I)=HUP(I, J)
HDN(J, I)=HDN(I, J)
300 Q
300 CONTINUE
C calculate the energy eigenvalues and wave vectors.
C
A = 1.0 - 0.9
CALL DMFSDO(OV,NB,A,IE1)
CALL DMTDS(HUP,NB,NR,OV,-1,IE2)
CALL DMTDS(HUP,NB,NR,OV,2,IE3)
CALL DMTDS(HDN,NB,NB,OV,-1,IE4)
CALL DMTDS(HDN,NB,NB,OV,2,IE5)
DO 7150 I=1,NB
DO 7150 J=1,I
IJ=I*(I-1)/2+J
T(IJ)=HUP(I,J)
7150 S(IJ)=HDN(I,J)
CALL DIGENT(I,X1,NB,0)
CALL DIGEN(S,X2,NB,0)
CALL DMTDS(X1,NB,NB,OV,1,IE6)
CALL DMTDS(X2,NB,NB,OV,1,IE7)
IF(IE1.EQ.0.AND.IE2.EQ.0.AND.IE3.EQ.0.AND.IE4.EQ.0.AND.IE5.EQ.0.
&.AND.IE6.EQ.0.AND.IE7.EQ.0) GO TO 5890
WRITE(6,5891) IE1,IE2,IE3,IE4,IE5,IE6,IE7
5891 FORMAT(1X,*IER=*,715)
STOP6
5890 CONTINUE
DO 7151 I=1,NB
IJ=I*(I-1)/2+I
XUP(I)=T(IJ)
7151 XDN(I)=S(IJ)
245 FORMAT(12F11.5)
WRITE(6,245) (XUP(J),J=NBST,NB)
PRINT 245
WRITE(6,245) (XDN(J),J=NBST,NB)
DO 357 II=1,NB
WRITE(2) XUP(II),(X1(JJ,II),JJ=1,NB)
357 WRITE(2) XDN(II),(X2(JJ,II),JJ=1,NB)
C calculate the density of states.
C
IF(NM.NE.1) GO TO 6532
AA=DMIN1(XUP(NBEND),XDN(NBEND))
XQ=AA-0.001
DO 2010 I=1,NEN
EN(I)=XQ
2010 XQ=XQ+DEN
6532 CONTINUE
  \( W_2 = W(NM)/SUMW \)
  DO 36 KK=NBST,NBEND
  DO 34 J=2,NEN
  \( M = J - 1 \)
  IF(XUP(KK).GT.EN(M).AND.XUP(KK).LE.FN(J)) GO TO 35
  34 CONTINUE
  SW(J)=SW(J)+WZ
  36 CONTINUE
  DO 336 KK=NBST,NBEND
  DO 334 J=2,NEN
  \( M = J - 1 \)
  IF(XDN(KK).GT.EN(M).AND.XDN(KK).LE.FN(J)) GO TO 335
  334 CONTINUE
  SW(J)=SW(J)+WZ
  336 CONTINUE
12000 CONTINUE
C
C DETERMINE THE FERMI ENERGY
C
  RH0=ELECT-18.D0
  A=0.0
  DO 39 J=1,NEN
  A=A+SW(J)
  39 TSW(J)=A
  NEN0=NEN-2
  DO 41 J=2,NEN0
  \( K = J - 1 \)
  IF(TSW(K).LT.RHO.AND.TSW(J).GE.RHO)GO TO 40
  41 CONTINUE
  WRITE(6,36741)
36741 FORMAT(1X,'FERMIE IS NOT CORRECT')
C
  GO TO 9999
  40 A=RH0-TSW(K)
  B=TSW(J)-RHO
  IF(A.LT.B) FERMIE=EN(K)
  IF(A.GE.B) FERMIE=EN(J)
  K1=K-20
  K2=K+20
  IF(K2.GT.NEN) K2=NEN
  DO 156 IOD=K1,K2
  WRITE(6,157) EN(IOD),SW(IOD),TSW(IOD)
  157 FORMAT(1X,A4,11X,F13.7))
  WRITE(6,158) FERMIE
  158 FORMAT(1X,'FERMI ENERGY=',F14.8,//)
  REWIND 1
RE*IND 2
381 DO 382 IRLV=1,KNMAX
     CKUP(IRLV)=0.00
     CKDN(IRLV)=0.00
     VKUP(IRLV)=0.00
382 VKDN(IRLV)=0.00
     NP3=NPGAUS*3
     DO 45 I=1,NP3
     COUP(I)=0.00
     CODN(I)=0.00
     VAUP(I)=0.00
     VADN(I)=0.00
45 CONTINUE
     DO 89998 NM=1,NKPT
     DO 358 II=1,NB
     READ(2) XUP(II),(XI(JJ,II),JJ=1,NB)
     READ(2) XDN(II),(X2(JJ,II),JJ=1,NE)
     CALCULATE FOURIER TRANSFORM OF CHARGE DENSITY
     DO 121 IRLV=1,KNMAX
     READ(1) SIJ
     AA=0.0
     CC=0.0
     DO 125 IN=NBST,NBEND
     IF(XONCIN*.GT.FERMI.GO TO 7125
     IJ=0
     DO 7122 I1=1,NB
     DO 7122 I2=1,I1
     IJ=IJ+1
     AC=X2(I1,IN)*SIJ(IJ)*X2(I2,IN)
     IF(I1.NE.I2)AC=AC*2.00
     7122 CC=CC+AC
     7125 CONTINUE
     IF(XUP(IN),.GT.FERMI.GO TO 125
     IJ=0
     DO 122 I1=1,NB
     DO 122 I2=1,I1
     IJ=IJ+1
     AC=X1(I1,IN)*STJ(IJ)*X1(I2,IN)
     IF(I1.NE.I2)AC=AC*2.00
     122 AA=AA+AC
     125 CONTINUE
     VKUP(IRLV)=VKUP(IRLV)+WT(NM)*AA
     VKDN(IRLV)=VKDN(IRLV)+WT(NM)*CC
     AA=0.00
BB=0.00
DO 6125 IN=NCST,NB
   IJ=0
   DO 6122 I1=1,NB
   DO 6122 I2=1,II
      IJ=IJ+1
      AC=X1(I1,IN)*SIJ(IJ)*X1(I2,IN)
      BC=X2(I1,IN)*SIJ(IJ)*X2(I2,IN)
   IF(I1.EQ.12) GO TO 612*
      AC=AC*2.00
      BC=BC*2.00
   6124 AA=AA+AC
   6122 BB=BB+BC
   6125 CONTINUE
   CKUP(IRLV)=CKUP(IRLV)+WT(NM)*AA
   CKDN(IRLV)=CKDN(IRLV)+WT(NM)*BB
   121 CONTINUE
C
C   CALCULATE SPHERICALLY AVERAGED CHARGE DENSITY
C
C   THE BASIS FUNCTION (BAS) IS CALCULATED IN PROGRAM 5.
C
PCONST=WT(NM)/SUM
IQ=0
DO 831 IR=1,NPGAUS
   DO 832 LDIR=1,3
   IQ=IQ+1
   SUPCO=0.00
   SDNCO=0.00
   SUPVA=0.00
   SDNVA=0.00
   NPTOL=NPUM(LDIR)
   PCON=PCONST/FLOAT(NPTOL)
   DO 833 LP=1,NPTOL
      READ(17) BAS
      DO 811 I=NCST,NB
         SS=(0.00,0.00)
         TT=(0.00,0.00)
         DO 812 J=1,NB
            SS=SS+XI(J,I)*BAS(J)
            TT=TT+X2(J,I)*BAS(J)
      812 CONTINUE
      SUPCO=SUPCO+CABS(SS)**2
      SDNCO=SDNCO+CABS(TT)**2
   811 CONTINUE
   DO 805 I=NBST,NBEND
      IF(XUP(I).GT.FERMIE) GO TO 821
SS=(0.00,0.00)
DO 806 J=1,NB
806 SS=SS*X1(J,1)*BAS(J)
SUPVA=SUPVA+CABS(SS)**2
821 IF(XDN(I).GT.FERMI) GO TO 805
TT=(0.00,0.00)
DO 807 J=1,NB
807 TT=TT*X2(J,1)*BAS(J)
SDNVA=SDNVA+CABS(TT)**2
805 CONTINUE
833 CONTINUE
COUP(IQ)=COUP(IQ)+SUPCO*PCON
CODN(IQ)=CODN(IQ)+SDNCO*PCON
VAUP(IQ)=VAUP(IQ)+SUPVA*PCON
VADN(IQ)=VADN(IQ)+SDNVA*PCON
832 CONTINUE
831 CONTINUE
89998 CONTINUE
WRITE(6,223)
C
THE SPHERICALLY AVERAGED CHARGE DENSITY IS APPROXIMATED AS THE ZEROTH
C ORDER TERM IN A SIX ORDER KUBIC HARMONIC EXPANSION.
C
IQ=0
DO 837 IR=1,NPGAUS
DENUP(IR)=0.0
DENDN(IR)=0.0
DO 838 LDIR=1,3
IQ=IQ+1
DENUP(IR)=DENUP(IR)+(COUP(IQ)+VAUP(IQ))*WTDIR(LDIR)
DENDN(IR)=DENDN(IR)+(CODN(IQ)+VADN(IQ))*WTDIR(LDIR)
834 FORMAT(5E15.8,15)
IF(IPUN.NE.0) WRITE(7,834) R(IR),COUP(IQ),VAUP(IQ),CODN(IQ),VADN(I
EQ),LDIR
838 CONTINUE
II=(IR-1)*3
WRITE(6,839) R(IR),DENUP(IR),DENDN(IR),(COUP(I1+J),CODN(I1+J),VAUP
L(I1+J),VADN(I1+J),J=1,3)
837 CONTINUE
839 FORMAT(IX,F5.2,14F9.3)
AA=(CKUP(1)+VKUP(1)-CKDN(1)-VKDN(1))/SUMW
RHO=(CKUP(1)+VKUP(1)+CKDN(1)+VKDN(1))/SUMW
WRITE(6,1780) AA,RHO
1780 FORMAT(/,1X,'MAGNETON NUMBER =',F13.7,'RHO=',F16.8,'1H1)
C
C MODIFIED THE SELF-CONSISTENT CORRECTIONS TO IMPROVE CONVERGENCE.
DO 378 KN=1,KNMAX
CADS=1.0/CON(KN)/OMEGA/SUMW
CKUP(KN)=CKUP(KN)*CADS
CKDN(KN)=CKDN(KN)*CADS
VKUP(KN)=VKUP(KN)*CADS
VKDN(KN)=VKDN(KN)*CADS
DKUP(KN)=DKUP(KN)+VKUP(KN)
DKDN(KN)=DKDN(KN)+VKDN(KN)

IF (IPUN.NE.0) WRITE(7,5643) IX(KN),IY(KN),IZ(KN),CKUP(KN),CKDN(KN)
& VKUP(KN),VKDN(KN)
5643 FORMAT(3I3.5X,F15.8)
89437 FORMAT(3I3.5X,F15.8)
WRITE(6,89437) IX(KN),IY(KN),IZ(KN),CKUP(KN),CKDN(KN),VKUP(KN),
& VKDN(KN)
VMSUP(KN)=DKUP(KN)
VMSDN(KN)=DKDN(KN)
378 CONTINUE
WRITE(6,223)
223 FORMAT(6,223)
WRITE(6,89413) ITER,FACT
89413 FORMAT(6,89413) ITER,FACT

C CALCULATE THE CORRECTION TO THE COULOMB PART OF V(K=0).

AA=0.00
RO2=RO*RO
RO3=RO*RO2
DO 451 J=2,KNMAX
RK1=RK(J)
RK2=RK1*RK1
RK3=RK1*RK2
RK4=RK2*RK2
RK5=RK*RK1

AA=AA+(DK(J)-VKUP(J)-VKDN(J))/RK1*((3.0*RO2/RK2-6.0/RK4)*DSIN(RK
& 5)+6.0*RO/RK3-3.0/RK1)*DCOS(RK1))*CON(J)
451 CONTINUE

C CALCULATE THE CORRECTION TO THE EXCHANGE POTENTIAL BY NUMERICAL GAUSSIAN INTEGRATION.

DO 401 I=1,NPGAUS
VUPR(I)=(DENUP(I)**ONETHD-DUP(I)**DNFTHD)*SIXPI
$\text{VDNR}(i) = (DENDN(i) ** \text{ONE THD} - DDN(i) ** \text{ONE THD}) \times 6 \pi$

401 CONTINUE
EXUP(1) = 0.0
EXDN(1) = 0.0
CC = 2.0 * PI * R0 / OMEGA
DO 403 I = 1, NPGAUS
EXUP(I) = EXUP(1) + W(I) * VUPR(I) * R(I) * R(I)
EXDN(I) = CC * EXUP(I)
DO 403 I = 1, NPGAUS
EXDN(I) = EXDN(1) + W(I) * VDNR(I) * R(I) * R(I)
FXDN(I) = CC * EXDN(I)
DO 404 J = 2, KNMAX
FXDN(J) = FXDN(1) + W(J) * VDNR(I) * R(I) * R(I)
FXUP(J) = FXUP(1) + W(I) * VUPR(I) * R(I) * R(I)
FXUP(J) = CC * FXUP(I)
DO 404 J = 2, KNMAX
FXDN(J) = FXDN(1) + W(J) * VDNR(I) * R(I) * R(I)
FXUP(J) = FXUP(1) + W(I) * VUPR(I) * R(I) * R(I)
DO 404 CONTINUE
WRITE (6, 32211)
ANUCLE = 0.0
DO 397 J = 1, KNMAX
IF (J .EQ. 1) GO TO 33397
DK(J) = -DK(J) / RKK(J) - VK0(J)
ANUCLE = ELECT / RKK(J) / OMEGA
33397 WRITE (6, 100) IX(J), IY(J), IZ(J), ANUCLE, VX0UP(J), VX0DN(J), VXUP(J), VXDN(J), EXUP(J), EXDN(J)
56802 FORMAT (5E14.8)
50100 FORMAT (5A4)
VX0UP(J) = EXUP(J)
VX0DN(J) = EXDN(J)
VK(J) = DK(J)
397 CONTINUE
100 FORMAT (IX, 12, 2I1, 12(IX, F9.5))
WRITE(19) (DK(I), DKUP(I), DKDN(I), EXUP(I), EXDN(I), I = 1, KNMAX)
WRITE (6, 223)
223 FORMAT (1H1)
9998 CONTINUE
REWIND 1
REWIND 2
REWIND 4
REWIND 17
PROGRAM 7. THE CENTRAL CELL INTEGRALS OF THE SPIN-ORBIT COUPLING, 
(P-P AND D-D BLOCKS)

******************************************************************************

** A = LATTICE CONSTANT (IN A. U.) 
** SC0= IDCUB=1, BCCO IDCUB=2. FCCO IDCUB=4 
** EXPVG= CONVERGENT CRITICAL DEXP(-EXPCVG)=0.00 
** ELECT=NUMBER OF ELECTRONS PER ATOM 
** K2MAX= THE SQUARE OF THE MAXIMUM MAGNITUDE OF THE RECIPROCAL LATTICE 
** VECTORS USED 
** KREAD=NO OF FOURIER COEFFICIENTS READ IN (1) 
** NKPT=DIMENSION OF KXX ECT. MUST BE GREATER THAN NO OF R.L.V. GENERATED 
** IC0BNO=GTO NUMBERS FOR & SYMMETRY 
** I&ATOM=ATOMIC BASIS NUMBER =0 IF INDEPENDENT GTO IS EMPLOYED 

IMPLICIT REAL *6 (A-F,H,O-Z) 
DIMENSION PP(3,3),VC0(1920),RK2(1920),DC0(3,3),GC0UL(4801) 
COMPLEX*16 AO,A1,A2,A3,A4 
DIMENSION R(96),W(96),Y(96) 
DIMENSION S8(25,25,3) 
DIMENSION H(10,10),X(10,10),T(55),YUP(10),OD(5) 
COMMON/GTO/CRYATL,PI,ISATOM,IPATOM,IDATOM 
COMMON/LCS/KXX,KKY,KKZ,NB,KSQU 
INTEGER*2 KXX(8184),KKY(8184),KKZ(8184),NR(8184) 
DIMENSION LILS(14),ALP(11),ALD(5),CS(14),CP(11),CD(5),SC0(4,14), 
PP(3,11),DC0(5,5) 
DIMENSION KSSQU(8184) 
1 FORMAT(A8,3F11.5,B5) 
READ(5,1) CRYSTL,A,ELECT,EXPCVG,IDCUB,NKPT,K2MAX,KREAD 
READ(5,4) ISOBNO,ISATOM,IPOBNO,IPATOM,IDOBNO,IDATOM 
WRITE(6,3) CRYSTL,A,ELECT,EXPCVG,IDCUB,NKPT,K2MAX,KREAD,ISOBNO,ISA 
ATOM,IPOBNO,IPATOM,IDOBNO,IDATOM 
3 FORMAT(I1X,A8,2X,'LATTICE CONST=',F10.5,2X,'ELECTRON NO=',F10.5,2X, 
1 'EXP MAX=',F10.5,2X,'ATOMS/LATTICE=',F15.2X,'NKPT=',I5,2X,'MAX K**2 
5=',I5,'/A**2,'K READ=',I5,5X, 
2 'SS=(','215',')**2X,*PP=',F215,*)&*2X,'OD=('','215','),')**2X,1/ 
LSMAX=ISOBNO 
LDMAX=IDOBNO 
LPMAX=IPOBNO 
IF(ISATOM.NE.0) LSMAX=ISATOM 
IF(IPATOM.NE.0) LDMAX=IPATOM 
IF(IPATOM.NE.0) LPMAX=IPATOM 
1 FORMAT(915) 
PI=3.14159265358979300 
AKR=2.00*PI/A 
AKR2=AKR*AKR
$A_{\text{HALF}} = A/2.0$
$\Omega = A^{\ast \ast 3}/D\text{FLOAT}(ID\text{CUR})$
$ID\text{ATOM} = 1$

Defines the Gaussian exponents, normalization constants, and expansion coefficients

CALL ROGTO(ALS, ALP, ALD, CS, CP, CD, SCO, PCO, DCO, ISOBN0, LSNMAX, 5, IDOBNO, LPMAX, IDOBNO, LDMAX, 0)
CALL GINDPK(KXX, KKY, KKZ, KSOU, NKPT, I)CUB, K2MAX, NR, 1, 1)
DO 23 J=1, KREAD
23 READ(1, END=22) GCOUL(J), GEX, GFUP, GFUPN, K2
22 CONTINUE
GCOUL(1) = -0.16074696D+01

D-D

CD1 = 1.0
CD2 = CD1/2.0
CD3 = CD2/DSQRT(3.0)
LDEN = 5*LDMAX
DO 534 L = 1, 3
DO 534 I = 1, LDEND
DO 534 J = 1, LDEND
534 SB(I, J, L) = 0.0
DO 25 I = 1, 10
DO 25 J = 1, 10
25 H(I, J) = 0.0
DOA = 0.0
DOB = 0.0
DO 45 K1 = 1, IDOBNO
DO 45 K2 = 1, IDOBNO
U = 1.0/(ALD(K1)+ALD(K2))
ALAMDA = ALD(K1)*ALD(K2)*U
DELTA = (PI*U)**1.5
U1 = ALD(K1)*U
U2 = ALD(K2)*U
CONST = U*DELTA*CD(K1)*CD(K2)/(8.00*ALD(K1)*ALD(K2))/3.00
CONST = CONST/274.074D0**2
C01 = CONST*U1*U2
C02 = -2.00*ALAMDA*CONST
C03 = C01*U2
C04 = C01*(2.00*U1-U2)
C05 = 2.00*C02
U0 = U/4.0
A = 0.0
DEFINE THE SPIN-ORBIT INTERACTION MATRICES BETWEEN ATOMIC FUNCTIONS
AND DIAGONALIZE IT WITH EIGENVALUE (XUP)
\[
\begin{align*}
H(1,4) &= DD\text{B} \\
H(1,7) &= DD\text{A} \\
H(1,8) &= -DD\text{A} \\
H(2,3) &= DD\text{A} \\
H(2,6) &= -DD\text{A} \\
H(2,9) &= -DD/2\text{D} \\
H(2,10) &= -DSQRT(3.00)/2\text{D}DD \\
H(3,6) &= -DD\text{A} \\
H(3,9) &= H(2,9) \\
H(3,10) &= -H(2,10) \\
H(4,7) &= H(2,9) \\
H(4,8) &= -H(2,9) \\
H(5,7) &= H(2,10) \\
H(5,8) &= H(2,10) \\
H(6,9) &= -DD\text{B} \\
H(7,8) &= -DD\text{A} \\
DO 125 I=1,10 \\
\text{DO 125 } J=1, I \\
IJ=I*(IJ-1/2)+J \\
125 \ T(IJ)=H(J,I) \\
\text{CALL DIGEN}(T, X1, 10, 0) \\
\text{DO 7151 } I=1,10 \\
\text{J}=I*(I-1)/2+I \\
\text{XUP}(I)=T(J) \\
7151 \text{ CONTINUE} \\
M=10 \\
85 \text{FORMAT}(1\text{H1}) \\
189 \text{FORMAT}(1\text{X},12.9(2\text{X},E12.6)) \\
86 \text{FORMAT}(1\text{X},//) \\
89 \text{FORMAT}(3\text{X},9\text{F14.6}) \\
I1=1 \\
71 \text{I2=I1+8} \\
\text{IF}(I2>W) I2=W \\
\text{WRITE}(6,85) \\
\text{WRITE}(6,89) (\text{XUP}(J), J=11,12) \\
\text{WRITE}(6,86) \\
\text{DO 72 I=1,M} \\
72 \text{WRITE}(6,189) I,(X1(I,J), J=11,12) \\
I1=I2+1 \\
\text{IF}(I2>W) \text{GO TO } 71 \\
\text{P-P} \\
\text{FINDS THE ASYMPTOTIC EXPRESSION FOR THE FOURIER COEFFICIENTS OF THE COULOMB POTENTIAL}
\end{align*}
\]
DEFINITE CONSTANTS TO PERFORM 96 POINTS GAUSSIAN INTEGRATION FOR LARGE VALUE OF THE RECIPROCAL LATTICE VECTORS

CALL GWTGAS196,Y,R,W)
STN=DSQRT(AKR2*DFLOAT(KSQU(NKPT))))
DEN=50.*DO*AKR
M=0
DO 901 I=1,20
DO 902 J=1,96
M=M+1
RK=DEN*RI(J)/2.DO+(2.DO*STN-DEN)/2.DO
RKS=RK*RK
VCO(M)=VCO(J)/RKS+VKC1/(RKS*(RKS+VKC2)**2)
902 CONTINUE
STN=STN+DEN
901 CONTINUE
DO 533 N=1,LPMAX
DO 533 M=1,LPMAX
PP(N,M)=0.DO
DO 40 K1=1,IPDBNO
DO 40 K2=1,IPDBNO

VCO0=-8.DO*PI*ELECT/DEMEGA
K1=KSQU(NKPT)
K2=K1-100
K3=K1-50
GK1=FLOAT(K1)*AKR2
GK2=FLOAT(K2)*AKR2
GK3=FLOAT(K3)*AKR2
AA=AK1*GCoul(K1+1)-VCO
BB=AK2*GCoul(K2+1)-VCO
AA=DSQRT(AA)
BB=DSQRT(BB)
VKC2=AA*(GK1-GK2)/(BB-AA)-GK2
VKC1=(AA*(GK1*VKC2))**2
VTEST=VCO/GK3+VKC1/(GK3*(GK3+VKC2)**2)
WRITE(6,50) VKC1,VKC2,K3,GCoul(K3+1),VTEST
50 FORMAT(1E16.8,1X,F16.8)
C1=VKC1/AKR2**3
C2=VKC2/AKR2
C3=VCO/AKR2
WRITE(6,58210) C1,C2,C3
58210 FORMAT(3F20.5)
U=1.D0/(ALP(K1)+ALP(K2))
ALPMA=ALP(K1)*ALP(K2)*U
DELTA=(PI*U)**1.5
CONST1=U/2.D0*DELTA/(274.07400**2)*CP(K1)*CP(K2)
CONST2=CONST1*DEN/2.00*OMEGA/(6.00*PI*PI)
DO 201 I=1,LPMAX
DO 201 J=1,LPMAX
201 CDC(I,J)=PCO(I,K1)*PCO(J,K2)
UOV4=U/4.D0
CENT1=0.D0
C
SUM OVER THE R.L.V. UP TO NKPT

DO 500 J=1,NKPT
EXPB=UOV4*AKR2*KSQU(J)
IF(EXPB.GT.EXPCVG) GO TO 400
KK=KSQU(J)+1
ADEL=DEXP(-EXPB)
CENT1=CENT1+ADEL*GCOUL(KK)*AKR2*DFLOAT(KSQU(J))*NB(J)/3.D0
500 CONTINUE
400 CONTINUE
CENT1=CENT1*CONST1
C
INTEGRATE FORM NKPT TO CONVERGNT

A=0.D0
DO 801 I=1,1920
EXPB=RK2(I)*U/4.D0
IF(EXPB.GT.EXPCVG) GO TO 801
ADEL=DEXP(-EXPB)
A=A+ADEL*VCOU(I)
801 CONTINUE
CENT2=CONST2*A
DO 408 I=1,LPMAX
DO 408 J=1,LPMAX
408 PP(I,J)=PP(I,J)+(CENT1+CENT2)*CDC(I,J)
CENT3=CENT1+CENT2
WRITE(6,9) K1,K2,CENT1,CENT2,CENT3
9 FORMAT(1X.2I5.3C2X.E14.8))
40 CONTINUE
PRINT 54802
54802 FORMAT(1HI)
LPST=LPMAX*5+LSMAX
DO 300 I=1,LPMAX
DO 300 J=1,LPMAX
II=LPST+3*(I-1)
JJ = LPST + 3*(J-1)
IX = I1 + 1
IY = I1 + 2
IZ = I1 + 3
JX = JJ + 1
JY = JJ + 2
JZ = JJ + 3
BB = PP(1, J)
A0 = (0.00, 0.00)
A1 = DCMPLX(0.00, BB)
A2 = -A1
A3 = DCMPLX(0.00, BB)
A4 = -A3
WRITE (6, 1023) IX, JY, A3, A0
WRITE (7, 1023) IX, JY, A3, A0
WRITE (6, 1023) IX, JZ, A0, A2
WRITE (7, 1023) IX, JZ, A0, A2
WRITE (6, 1023) IY, JX, A4, A0
WRITE (7, 1023) IY, JX, A4, A0
WRITE (6, 1023) IY, JZ, A0, A3
WRITE (7, 1023) IY, JZ, A0, A3
WRITE (6, 1023) IZ, JX, A0, A1
WRITE (7, 1023) IZ, JX, A0, A1
WRITE (6, 1023) IZ, JY, A0, A4
WRITE (7, 1023) IZ, JY, A0, A4
300 CONTINUE
1023 FORMAT (2I5, 4E15.8)
STOP
END
**PROGRAM 8. ENERGY BANDS INCLUDING THE EFFECTS OF SPIN-ORBIT COUPLING**

********************************************************

**CALCULATE THE ENERGY EIGENVALUES (E) AND EIGENVECTORS (X)**

\[ HX = SE \]

**THE OVERLAP MATRIX (S) IS EXPRESSED AS THE PRODUCT OF A UPPER TRIANGULAR MATRIX (R) AND ITS TRANSPOSE (R\(^T\))**

\[ H^*X = X^*E, \quad \text{WHERE} \quad H^* = ((R\,**T\)**-1)H(R\,**-1) \quad \text{AND} \quad X^* = RX \]

********************************************************

**COMPLEX*16 H,X,DCONJG**

**COMPLEX*8 Y(76,76),GN,CMPLX,CONJG**

**REAL*8 E(76),FUP(36),W(76),OV,EPS**

**DIMENSION GUP(741),GDN(741),GOV(741),FIG(76),DUP(36)**

**DIMENSION INDEX(76)**

**COMMON/LCS/GNI (38.38),GM1(38.38)**

**COMMON/A/H(76,76)**

**COMMON/B/X(76,76)**

**COMMON/C/OV(2926)**

**EQUIVALENCE (H(1,1),Y(1,1)),(H(1,39),FUP(1))**

**EQUIVALENCE (X(1,1),GUP(1)),(X(1,26),GDN(1)),(X(1,51),GOV(1))**

**78210 FORMAT(215)**

**COMM.**

**FIND E AND X FOR K=KST TO KEND**

**IF(IWRITE,NE,0) RESULTS ARE PRINTED**

**READ(5,78210) KST,KEND,WRITE**

**DO 2 J=1,38**

**DO 2 I=1,38**

**GNI(I,J)=0.DO**

**GN(I,J)=CMPLX(GC,GD)**

**CONTINUE**

**2 CONTINUE**

**10 FORMAT(215.4E15.8)**

**READ IN SPIN-ORBIT MATRIX (OUTPUT OF PROGRAM 7)**

**DO 1 N=1,706**

**READ(5,10) END=9 I,J,GA,GB,GC,GD**

**GNI(I,J)=GB**

**GN(I,J)=CMPLX(GC,GD)**

**CONTINUE**

**9 CONTINUE**

**M=76**

**KK=KST-1**

**DO 74239 KPT=1,KK**

**READ(1) GX,GY,GZ,WEIGT,(EIG(I),I=1,M),(DUP(J),J=1,36)**

**DO 74239 I=1,M**
DEFINE THE HAMILTONIAN AND OVERLAP MATRICES

DO 56940 KPT=1,KEND
READ(2) GX,GY,GZ,WEIGT,(GUP(I),GDN(I),I=1,741)
READ(3) GX,GY,GZ,WEIGT,(GOV(I),I=1,741)
IF(KPT.LE.KST) GO TO 56940
DO 15 I=1,38
   J=I+38
   DO 15 J=I,38
   JJ=J+38
   IJ=J*(J-1)/2+I
   H(I,J)=CMPLX(GUP(IJ),GMI(I,J))
   G=-GMI(I,J)
   H(IJ,J)=CMPLX(GDN(IJ),G)
   OV(I,J)=DBLE(OV(IJ))
   15 CONTINUE

DMFSD REPLACE OV BY AN UPPER TRIANGULAR MATRIX R WHERE OV=(R**T)*R
DMFSD IS IN IBM SCIENTIFIC SUBROUTINE PACKAGE

CALL DMFSD(OV,38,1,0.7,IFR)
IF(IFR.NE.0) GO TO 7200
GO TO 300

7200 CONTINUE

DIGEN DIAGONALIZED MATRIX OV
DIGEN IS THE DOUBLE PRECISION VERSION OF SUBROUTINE EIGEN IN IBM S,S,P.

CALL DIGEN(OV,GMI,38,0)
DO 55 I=1,38
   J=I+(I-1)*1/2
   WRITE(6,57) OV(J)
   55 CONTINUE

57 FORMAT(5X,11(F10.7,1X))
STOP 5

300 CONTINUE
DO 19 I=1,38
   J=I+1
   IJ=J*(J-1)/2+J
   IJJJ=(I+38)*(I+37)/2+J+38
   OV(IJJJ)=OV(IJ)
   19 CONTINUE
DO 11 J=39,76
   IJ=J*(J-1)/2+I
J  J  =J - 38
H(I,J)=G(N(I,JJ)
OV(IJ)=0.DO
11 CONTINUE
DO 12 I=1,76
DO 12 J=1,1
H(I,J)=DCONJG(H(J,I))
12 CONTINUE

SUBROUTINE HRIN TRANSFORM H INTO H (R**-1)
SUBROUTINE RTINH TRANSFORM H INTO ((R**T)**-1) H
CALL HRIN(M)
CALL RTINH(M)

CEIGD DIAGONALIZE A COMPLEX HERMITIAN MATRIX H WITH FIGFNVALUE E AND EIGENVECTORS X (NOT INCLUDED IN THIS THESIS)
IND=1
EPS=1.D-7
CALL CEIGDP(H,X,E,M,EPS,9000,ITER,IND,INDEX,M)

DEFINE PROJECTION OPERATOR FOR MAJORITY SPIN

DO 800 I=1,36
800 FUP(I)=0.0
DO 810 I=1,36
DO 810 K=1,38
810 FUP(I)=FUP(I)+CDABS(X(K,I))**2
DO 820 I=1,36
820 DUP(I)=FUP(I)

SUBROUTINE FUNCT TRANSFORM EIGENVECTORS X INTO (R**-1) X
CALL FUNCT(M)
DO 76581 I=1,M
EIG(I)=E(I)
DO 76581 J=1,M
Y(I,J)=X(I,J)
76581 CONTINUE
56081 CONTINUE
53405 FORMAT(1X,'K=(*,3F6.2,*),5X,'ITERATION=',5X,'IND=',5X,'NM=',5X,'WEIGHT=',F10.4)
M=76
WRITE(1) GX,GY,GZ,WEIGT,(EIG(I),I=1,M),(DUP(J),J=1,36)
DO 76539 I=1,M
WRITE(1) (Y(J,I), J=1,M)
76539 CONTINUE
WRITE(6,53405) GX, GY, GZ, ITER, IND, KPT, WIGHT
IF(IPRINT.EQ.0) GO TO 56940
85 FORMAT(1H1)
86 FORMAT(1X,//)
I2=0
71 CONTINUE
11=12+1
12=12+5
IF(12.GT.M) I2=M
88 FORMAT(5(8X,I10,8X))
WRITE(6,86)
WRITE(6,88) (I, I=11,12)
WRITE(6,86)
WRITE(6,89) (E(I), I=11,12)
WRITE(6,86)
IF(I2.LE.36) WRITE(6,89) (DUP(I), I=11,12)
WRITE(6,86)
89 FORMAT(3X,5(6X,F14.7,6X))
189 FORMAT(1X,12,10(1X,E12.6))
DO 72 I=1,M
72 WRITE(6,189) I, (X(I,J), J=11,12)
WRITE(6,85)
IF(I2.LT.46) GO TO 71
56940 CONTINUE
STOP
END
PROGRAM 9. THE MOMENTUM MATRICES BETWEEN BAND STATES.

SUM CONJG(X(I,N,K))*P(I,J,K)*X(J,M,K) OVER ALL STATES I & J.
WHERE X IS EIGENVECTOR AT K IN B. Z.
P IS THE MOMENTUM MATRIX BETWEEN BASIS BLOCH STATES. (PROGRAM 2 & 4)

COMPLEX*16 X(76,12), CX(76,12), BX(78), BY(78), BZ(78), A, SX, SY, SZ
COMPLEX*8 F(76,76), SBX(78), SBY(78), SBZ(78)
DIMENSION E(76), PX(741), PY(741), PZ(741)
DIMENSION FUP(36)
COMMON/LCS/F
4 FORMAT(4I5)

CALCULATE FOR K FROM NKST TO NKEND
RESULTS ARE PRINTED IF (IPRIT.NF.0)

READ(5,4) NKST,NKEND, IPRIT
DO 999 NMK=I,NKEND

READ IN ENERGY ADN WAVE VECTOR. (OUT PUT OF PROGRAM 8)

READ(1) XK,YK,ZK,WT,(E(I),I=1,76),(FUP(I),I=1,36)
DO 10 I=1,76
10 READ(1) (F(J,I),J=1,76)
199 CONTINUE

READ IN MOMENTUM MATRIX BETWEEN BASIS BLOCH STATES. (PROGRAMS 2 & 4)

READ(2) XL,YL,ZL,(PX(I),I=1,741)
READ(2) XL,YL,ZL,(PY(I),I=1,741)
READ(2) XL,YL,ZL,(PZ(I),I=1,741)
IF(XK.NE.XL.OR.YK.NE.YL.OR.ZK.NE.ZL) GO TO 199
IF(NMK.LT.NKST) GO TO 999
DO 40 I=1,76
DO 40 J=1,12
X(I,J)=F(I,J+18)
40 CX(I,J)=DCONJG(X(I,J))
DO 20 I=1,78
BX(I)=(0.0D0,0.0D0)
BY(I)=(0.0D0,0.0D0)
BZ(I)=(0.0D0,0.0D0)
20 CONTINUE
DO 61 I=2,38
II=I+38
II=I-1
DO 61 J=1,IMX
   IJ=I*(I-1)/2+J
   JJ=J+38
   SX=CMPLX(PX(IJ),0.E0)
   SY=CMPLX(PY(IJ),0.E0)
   SZ=CMPLX(PZ(IJ),0.E0)
   NN=0
   DO 60 N=1,12
      DO 60 M=1,N
         NN=NN+1
         A=PX(IJ)*SX+PY(IJ)*SY+PZ(IJ)*SZ
         BX(NN)=BX(NN)+A*SX
         BY(NN)=BY(NN)+A*SY
         BZ(NN)=BZ(NN)+A*SZ
      60 CONTINUE
   61 CONTINUE
   DO 65 I=1,38
      II=(I+38)/2
      SX=CMPLX(PX(I),0.E0)
      SY=CMPLX(PY(I),0.E0)
      SZ=CMPLX(PZ(I),0.E0)
      NN=0
      DO 66 N=1,12
         DO 66 M=1,N
            NN=NN+1
            A=PX(I)*SX+PY(I)*SY+PZ(I)*SZ
            BX(NN)=BX(NN)+A*SX
            BY(NN)=BY(NN)+A*SY
            BZ(NN)=BZ(NN)+A*SZ
         66 CONTINUE
   65 CONTINUE
   DO 700 I=1,78
      SBX(I)=BX(I)
      SBY(I)=BY(I)
      SBZ(I)=BZ(I)
   700 CONTINUE
   WRITE(15) XK,YK,ZK,(SBX(I),SBY(I),SBZ(I),I=1,78)
   WRITE(6,59) NMK,XK,YK,ZK,WT
59 FORMAT(15,4(F14.5,3X),/)
   IF(IPRIT.EQ.0) GO TO 999
   DO 151 I=1,12
      DO 151 J=1,I
         IJ=I*(I-1)/2+J
         WRITE(6,152) I,J,SBX(IJ),SBY(IJ),SBZ(IJ)
   151 CONTINUE
152 FORMAT(1X,2I5,8(2X,F13.7))
PRINT 56194
56194 FORMAT(1H1)
999 CONTINUE
19999 STOP
END
**PROGRAM 10. THE DENSITY OF STATES**

**CALCULATE THE DENSITY OF STATES BY THE HYBRIDE METHOD**

ENERGY BANDS AND MOMENTUM MATRICES INCLUDING THE EFFECTS OF SPIN-ORBIT COUPLING ARE USED.

KL = DIVISION BETWEEN K = (0,0,0) AND K = 2*PI/A(1,0,0)

NB = NUMBER OF STATES CONSIDERED

A = LATTICE CONSTANT

E_MIN = MINIMUM OF ENERGY

N макс = TOTAL NUMBER OF POINTS WHERE DENSITY OF STATES NEED TO BE CALCULATED

D_E = STEP SIZE IN ENERGY

VALEL = NUMBER OF BAND ELECTRONS

DE_GCR = DEGENERATE CRITICAL VALUE USED IN K.P PERTURBATION THEORY

N_KPT = NUMBER OF POINTS IN THE BRILLIUMIN ZONE

N_ICUB = NUMBER OF ATOMS PER LATTICE

**DIMENSION** D_E (N_KSUM, N_B)

**COMPLEX** 8 P_X(12,12), P_Y(12,12), P_Z(12,12), S.PLJ, SPF, SPJ

**INTEGER** 2 N_P(18,18,18)

**DIMENSION** X(6), D_E (3,3), N_P (6)

**DIMENSION** E (5), W (5), E (12), I (5), N_A_B (9)

**DIMENSION** S_W (1003), S_W D N (1003), E N (1003), PLECT (1003)

**DIMENSION** F_UP (12), E_E (12)

**DIMENSION** D_E K_Z (2083,12)

**COMMON**/LCS/ D_E K X (2083,12), D_E K Y (2083,12)


**CALL** IDENT ('1103 40149 SHI')

**10 FORMAT** (215,5 F 10.5, 415)

READ (5, 10) KL, NB, A, E_MIN, DE, VALEL, DEGCR, N макс, N_KPT, N_KSUM, N_ICUB

**EPERC** = D FLOAT (ID CUB)

N_B_P_M = 2*N_A_B * 1

**DO 111 N = 1, N_B_P_M**

**WRITE** (6, 11) KL, NB, A, E_MIN, DE, VALEL, DEGCR, N макс, N_KPT, N_ICUB

**11 FORMAT** (1 H, 'KX-LENGTH=', I 2, 5X, 'NO. OF BANDS=', I 2, 5X, 'LATTICE CONSTA

**1 INT=', I 8, 5X, 'EMIN=', E 8, 5X, 'DE=', E 8, 5X, 'NO. OF EL=', F 4, 1, /

**27, 1X, 'DEG CRT=', E 8, 5X, 'NO OF DE=', E 8, 5X, 'NO OF Pt=', E 8, 5X, 'SUR D

**3 IV=', I 5, ')

PI = 3.141592653589793

PI KL = PI/KL

D I V N O = D FLOAT (MAXB P)


B = PI KL/A
READ MOMENTUM MATRICES AND DEFINE POINTS IN THE R, Z.

DO 1 NPT=1,NKPT
READ(1) XK,YK,ZK,(PX(I,J),PY(I,J),PZ(I,J),J=1,1),I=1,NB)
IF(KL*NE.8) GO TO 2351
XK=XK/2.0
YK=YK/2.0
ZK=ZK/2.0
2351 CONTINUE
I=IFIX(XK)+1
J=IFIX(YK)+1
K=IFIX(ZK)+1
NP(J,I,K)=NPT
NP(I,J,K)=NPT
DO 2 L=1,NB
DEKX(NPT,L)=2.0*REAL(PX(L,L))
DEKY(NPT,L)=2.0*REAL(PY(L,L))
DEKZ(NPT,L)=2.0*REAL(PZ(L,L))
2 CONTINUE
1 CONTINUE
REWIND 1
KLP2=KL*2

GENERATE ENERGY DERIVATIVES IN THE NEIGHBORING POINTS OF THE 1/16TH OF THE
BRILLIQUIN ZONE

CALL GNBDE(DEKX,DEKY,DEKZ,NKSUM,NB,NP,KLP2,NKPT)
DO 299 NE=1,NEMAX
SUMW(NE)=0.0
SWDN(NE)=0.0
EN(NE)=EWIN+DE*(NE-1)
299 CONTINUE
EMAX=EN(NEMAX)
SUMWT=0.0
NMPT=0
DO 310 NPT=1,NKPT

READ ENERGY AND PROJECTION OPERATOR FOR UP SPIN
READ(10) XK, YK, ZK, WTT, (E(L), FUP(L), L=1, NB)
KX=FIX(XK)
KY=FIX(YK)
KZ=FIX(ZK)
IF(KL, NE, 8) GO TO 319
KX=KX/2
KY=KY/2
KZ=KZ/2
319 CONTINUE
READ(1) XK, YK, ZK, (PX(I, J), PY(I, J), PZ(I, J), J=1, I), I=1, NB)
IF(KZ, NE, 0, AND, KX, NE, KY, AND, KZ, NE, KL) GO TO 310
DO 35 I=1, NB
DO 35 J=I, NB
PX(I, J)=CONJG(PX(J, I))
PY(I, J)=CONJG(PY(J, I))
PZ(I, J)=CONJG(PZ(J, I))
35 CONTINUE
SUBDIVIDE EACH CUBE IN THE B.Z. INTO 27 MINICELLS
NTEST=0
DO 400 IDZ=1, MAXBP
KDZ=MAXBP*KZ+NABP(IDZ)
IF(KDZ, LT, 0, OR, KDZ, GT, KLDIV) GO TO 400
KNZ=KZ+NABP(IDZ)+1
SKZ=FLOAT(NABP(IDZ))*BDIV*2.0
DO 401 IDY=I, MAXBP
KDY=MAXBP*KY+NABP(IDY)
IF(KDY, LT, 0, OR, KDY, GT, KLODIV) GO TO 401
KNY=KY+NABP(IDY)+1
SKY=FLOAT(NABP(IDY))*BDIV*2.0
DO 402 IDX=1, MAXBP
KDX=MAXBP*KX+NABP(IDX)
IF(KDX, LT, KDY, OR, KDX, GT, KLODIV) GO TO 402
KNX=KX+NABP(IDX)+1
SKX=FLOAT(NABP(IDX))*BDIV*2.0
400 CONTINUE
KTOL=KDX*KDY*KDZ
IF(KTOL, GE, KLDIV) GO TO 402
NBKPT=NP(KNX, KNY, KNZ)
NMPT=NMPT+1
CALL WFC16(KDX, KDY, KDX, KLDIV, WT)
SUMWT=SUMWT+WT
SSQ=SKX*SKX+SKY*SKY+SKZ*SKZ
LST=0
AA=WT*VNORM*16.0
DO 320 L = 1, NB
IF (L .LT. LST) GO TO 320
GDKX = DEKX(NPT, L)
GDKY = DEKY(NPT, L)
GDKZ = DEKZ(NPT, L)
ENG = E(L)
NDEG = 1
IF (SSQ .EQ. 0.0) GO TO 32
LP1 = L + 1
DELE = ABS(E(LP1) - E(L))
336 CONTINUE
IF (L .NE. NB .AND. DELE .LT. DFGCRT) GO TO 330
C
C CALCULATE ENERGY BY SECOND ORDER K·P PERTURBATION THEORY
C
ENG = ENG - SKX*GDKX + SKY*GDKY + SKZ*GDKZ + SSQ
DO 30 J = 1, NB
IF (L .EQ. J) GO TO 30
0E = E(L) - E(J)
SPLJ = SKX*PX(L, J) + SKY*PY(L, J) + SKZ*PZ(L, J)
ENG = ENG + 4.0*CABS(SPLJ)**2/DELE
30 CONTINUE
GDKX = DEKX(NPT, L) + (DEKX(NBKPT, L) - DEKX(NPT, L))/DIVNO
GDKY = DEKY(NPT, L) + (DEKY(NBKPT, L) - DEKX(NPT, L))/DIVNO
GDKZ = DEKZ(NPT, L) + (DEKZ(NBKPT, L) - DEKZ(NPT, L))/DIVNO
32 CONTINUE
FEW(L) = ENG
IF (ENG .GT. EMAX) GO TO 320
CONUP = AA*FUP(L)
CONDN = AA - CONUP
93 FORMAT (IH, 3F12.5, 2I10, 2I5, F14.6, 15, 2(2X, F14.8), 15)
GDKX = ABS(GDKX)
GDKY = ABS(GDKY)
GDKZ = ABS(GDKZ)
GDKM = SORT((GDKX*GDKX + GDKY*GDKY + GDKZ*GDKZ)
IF (GDKM .LT. 1.0E-06) GO TO 500
CALL DENSIT(SWUP, SWON, EN, EMAX)
GO TO 320
330 CONTINUE
C
C CALCULATE ENERGY BY DEGENERATE SECOND ORDER K·P PERTURBATION THEORY
C
DO 331 N = LP1, NB
331 IF (ABS(E(L) - E(N)) .LT. DEGCRT) NDEG = NDEG + 1
DO 332 N = 1, NDEG
NN = N + L - 1
DO 332 M=1,N
MM=M+L-1
HD(N,M)=2.0*(SKX*PX(NN,MM)+SKY*PY(NN,MM)+SKZ*PZ(NN,MM))
IF(N.NE.M) GO TO 333
HD(N,M)=HD(N,M)+E(NN)+SSQ

333 CONTINUE
DO 334 J=1,NB
IF(J.GE.L.AND.J.LT.L+NOEG) GO TO 334
DELE=(E(NN)+E(MM))/2.0-E(J)
SPNJ=SKX*PX(NN,J)+SKY*PY(NN,J)+SKZ*PZ(NN,J)
SPJM=SKX*PX(J,MM)+SKY*PY(J,MM)+SKZ*PZ(J,MM)
HD(N,M)=HD(N,M)+4.0*SPNJ*SPJM/DELE

334 CONTINUE
HD(M,N)=CONJG(HD(N,M))

332 CONTINUE
IUD=2

CEIG DIAGONALIZES A COMPLEX MATRIX (HD) WITH EIGENVALUE (FIG)
SUBROUTINE CEIG IS NOT INCLUDED IN THIS THESIS
CALL CEIG(HD,UX,EIG,NDEG,1.E-7,9000,ITER,IUD,WK,IND,5)
LST=L+NDEG
DO 329 N=1,NDEG
ENG=EIG(N)
LN=L+E(N)
GDKX=DEKX(NPT,LN)+(DEKX(NBKPT,LN)-DEKX(NPT,LN))/DIVNO
GDKY=DEKY(NPT,LN)+(DEKY(NBKPT,LN)-DEKY(NPT,LN))/DIVNO
GDKZ=DEKZ(NPT,LN)+(DEKZ(NBKPT,LN)-DEKZ(NPT,LN))/DIVNO
EEW(LN)=ENG
IF(ENG.GT.EMAX) GO TO 320
CONUP=AA*FUP(LN)
CONDN=AA-CONUP
GDKX=ABS(GDKX)
GDKY=ABS(GDKY)
GDKZ=ABS(GDKZ)
GDKM=SQRT(GDKX*GDKX+GDKY*GDKY+GDKZ*GDKZ)
IF(GDKM+LT.1.E-06) GO TO 500
CALL DENSIT(SWUP,SWDN,EN,NEMAX)
329 CONTINUE
GO TO 320
500 CONTINUE

CONTRIBUTION FROM CRITICAL POINTS ARE NEGLECTED
WRITE(6,84) GDKX,GDKY,GDKZ,NPT,KDX,KDY,KDZ,ENG,L,AA,CUP,NDEG
84 FORMAT(1H,3F12.5,2I10,2I5,F14.6,15,Z(2X,F14.8),15,2X,1HC)
IF (NDEG.NE.1 .AND. N.NE.NDEG) GO TO 329
CONTINUE
320

FORMAT(313,F7.4,2X,12F9.5)
WRITE(3) KDX,KDY,KDZ,W,T,(EEW(L),L=1,NB)
WRITE(6,88) KDX,KDY,KDZ,W,(EFW(L),L=1,NB)

CONTINUE
402

CONTINUE
401

CONTINUE
400

CONTINUE

IF(KX+KY+KZ.NE.KL*3/2-2 .OR. NTEST.NE.0) GO TO 310
NTEST=1
KDX=KZ*MAXBP+2
IF(KDX.LT.O.OR.KDX.GT.KLOI V) GO TO 310
KDY=KY*MAXBP+2
IF(KDY.LT.O.OR.KDY.GT.KLDIV) GO TO 310
KDX=KX*MAXBP+2
IF(KDX.LT.KDY.OR.KDX.GT.KLDIV) GO TO 310
SKZ=2.0*BDIV*2.0
SKX=SKZ
SKY=SKZ
WRITE(6,312) KDX,KDY,KDZ

FORMAT(310) GO TO 315
310

CONTINUE
WRITE(6,45) SUMWT,VNORM,B,NMPT

FORMAT(1HO,5X,'SUM OF WEIGHT=',E12.5,10X,'VNORM=',F12.3,10X,
=B=',F12.5,10X,'NO POINT=',I10)
76

WRITE(6,76)

998

DENHU=0.0
DENHD=0.0
DENC=0.0
DO 296 NE=1,NEMAX
DENHU=DENHU+SWUP(NE)*DE
DENHD=DENHD+SWDN(NE)*DE
SWT=SWUP(NE)+SWDN(NE)
ELECT(NE)=DENHU+DENHD
DMAG=DENHU-DENHD
WRITE(6,44) EN(NE),SWUP(NE),DENHU,SWDN(NE),DENHD,SWT,ELECT(NE),

6DMAG

CONTINUE
DO 11000 I=2,NEMAX
K=I-1
IF(ELECT(K).LT.VALEL.AND.ELECT(I).GT.VALEL)FERMIF=EN(I)-
=DE*(ELECT(I)-VALEL)/(ELECT(I)-ELECT(K))
1100 CONTINUE
WRITE(6,12351) FERMIE
12351 FORMAT(1X,/,1X,'FERMIE ENERGY=',F10.5)
NMAX2=NMAX+2
CALL SPLOTE(SWON,SWUP,EN,NMAX,EMIN,DE,FERMIE,NMAX2)
STOP
END
PROGRAM 11 THE INTERBAND OPTICAL CONDUCTIVITY TENSOR

* * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *

CALCULATE THE INTERBAND OPTICAL CONDUCTIVITY BY THE HYBRID METHOD

KL = DIVISION BETWEEN K = (0, 0, 0) AND K = 2*PI/A(1, 0, 0)
NB = NUMBER OF STATES STORED FOR THE MOMENTUM MATRICES
A = LATTICE CONSTANT
FMIN = MINIMUM OF ENERGY
NMAX = TOTAL NUMBER OF POINTS WHERE DENSITY OF STATES NEED TO BE CALCULATED
DE = STEP SIZE IN ENERGY
DEGCRT = DEGENERATE CRITICAL USED IN K.P PERTURBATION THEORY
NKPT = NUMBER OF POINTS IN THE BRILLOUIN ZONE
FPERC = NUMBER OF ATOMS PER LATTICE

DIMENSION PXPX(NKDOM, NB), ECT

* * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *

COMPLEX*8 PX(78), PY(78), PZ(78)
INTEGER*2 NPI(18, 18, 18), KXX(1357), KYY(1357), KZZ(1357)
DIMENSION SWX(352), SWY(352), SWZ(352), EN(352), SWJON(352)
DIMENSION EE(12), DE(12), DEX(12), DEY(12), DEZ(12)
DIMENSION NABP(3)
DIMENSION PZPZ(2078, 12)
COMMON/LCS/PX(78), PY(78), PZ(78)
COMMON/AR/FNG, GDKX, GDKY, GDKZ, GDKM, B2, BDIV, CONXX, CONXY, CONZZ, CONST
READ(5, 10) KL, NB, A, FMIN, DE, FERMIE, DEGCRT, NMAX, NKPT, NKSUM

10 FORMAT(2IS5, SF10.5, 4IS5)

NABPMX = 1
MAXBP = 2*NABPMX + 1
DO 111 N = 1, MAXBP
111 NABP(N) = N - NABPMX - 1
KLDIV = KL*MAXBP
MAXBP = 1
WRITE(6, 11) KL, NB, A, FMIN, DE, FERMIE, DEGCRT, NMAX, NKPT, MAXBP, NKSUM
11 FORMAT(1H, 'KX-LENGTH=', I2, 5X, 'NO. OF BANDS=', I2, 5X, 'LATTICE CONSTA
27X, 'DEG CRIT=', F7.5, 5X, 'NO OF DE=', I5, 5X, 'NO OF PT=', I5, 5X, 'SURD
31V=', I5, 5X, 'DIM K PTS=', I5, 5)
PI = 3.141592653589793
PIKL = PI/KL
DIVNO = FLOAT(MAXBP)
VNORM = (A/12.*PI)**3/4.
B = PIKL/A
BDIV = B/DIVNO
KLD2 = KLDIV/2
TWOB = B*2.0
B2 = BDIV*BDIV
KLMAX = KLDIV*3/2
READ MOMENTUM MATRICES AND ORDER POINTS IN THE B. Z.

DO 1 NPT=1,NKPT
READ(1) XK,YK,ZK,(PX(I),PY(I),PZ(I),I=1,78)
1 IF(KL,NE,A) GO TO 2351
XK=XK/2.0
YK=YK/2.0
ZK=ZK/2.0
2351 CONTINUE
I=IFIX(XK)+1
J=IFIX(YK)+1
K=IFIX(ZK)+1
KXX(NPT)=I-1
KYY(NPT)=J-1
KZZ(NPT)=K-1
NP(I,J,K)=NPT
NP(J,I,K)=NPT
1 CONTINUE
REWIND 1
DO 299 NE=1,NEMAX
SWXX(NE)=0.0
SWXY(NE)=0.0
SWZZ(NE)=0.0
SWJON(NE)=0.0
EN(NE)=EMIN+DE*(NE-1)
299 CONTINUE
EMAX=EN(NEMAX)
MAXBP=3
DO 311 LG=1,NB
DO 30 NPT=1,NKPT
READ(1) XK,YK,ZK,(PX(I),PY(I),PZ(I),I=1,78)
30 LL=1,LG
I=LG*(LG-1)/2+LL
PXPX(NPT,LL)=REAL(PX(IJ)*CONJG(PX(IJ))+PY(IJ)*CONJG(PY(IJ)))*8.0
PZPZ(NPT,LL)=REAL(PZ(IJ)*CONJG(PZ(IJ))+PZ(IJ)*CONJG(PZ(IJ)))*8.0
PXPY(NPT,LL)=AIMAG(PX(IJ)*CONJG(PY(IJ)))*16.0
311 CONTINUE
DEFINE NEIGHBORING POINTS FOR K LIES ON THE SURFACE OF 1/16TH OF THE B. Z.

KLP2=KL+2
CALL GNAPPT(PXPX,PXPY,PZPZ,NKSUM,NB,NP,KLP2,NKPT,LG)
SUMWT=0.0
NMPT=0
NCRIT=0
DO 310 NPT=1,NKPT
   KX=KXX(NPT)
   KY=KYY(NPT)
   KZ=KZZ(NPT)
   NTST=0
SUBDIVIDE EACH CUBE IN THE B, Z, INTO 27 MINICELLS

DO 400 IDZ=1,MAXBP
   KDZ=MAXBP*KZ+NABP(IDZ)
   IF(KDZ.LT.0. OR.KDZ.GT.KLDIV) GO TO 400
   KNZ=KZ+NABP(IDZ)+1
   SKZ=FLOAT(NABP(IDZ))*BDIV*2.0
   DO 401 IDY=1,MAXBP
      KDY=MAXBP*KY+NABP(IDY)
      IF(KDY.LT.0. OR.KDY.GT.KLDIV) GO TO 401
      KNY=KY+NABP(IDY)+1
      SKY=FLOAT(NABP(IDY))*BDIV*2.0
   DO 402 IDX=1,MAXBP
      KDX=MAXBP*KX+NABP(IDX)
      IF(KDX.LT.KDY OR.KDX.GT.KLDIV) GO TO 402
      KNX=KX+NABP(IDX)+1
      SKX=FLOAT(NABP(IDX))*BDIV*2.0
315 CONTINUE
   KTOL=KDX*KDY*KZ
   IF(KTOL.GT.KLDMAX) GO TO 402
   NBKP=NP(KNX,KNY,KNZ)
   NMPT=NMPT+1
READ IN ENERGIES AND ENERGY DERIVATIVES CALCULATED IN PROGRAM 10.
READ(2) NDX,NDY,NDZ,WT,(EE(I),DFX(I),DEY(I),DEZ(I),I=1,NB)
   SUMWT=SUMWT+WT
   SSQ=SKX*SKX+SKY*SKY+SKZ*SKZ
   CONXX=PXPX(NPT,LL)*WT
   GDKM=SORT(DFX(1)*DFX(1)*DEY(1)*DEY(1)*DEZ(1)*DEZ(1))
   IF(GDKM.LT.1.E-5) NCRIT=NCRIT+1
   IF(SSQ.NE.0.0) GO TO 402
DO 320 LL=1,GB
   IF(EE(LL).LT.FERMIE.OR.EE(LL).GT.FERMIE) GO TO 320
   ENG=EE(LL)-EE(LL)
   IF(ENG.GT.EMAX) GO TO 320
   GDXX=ABS(DFX(LL)-DFX(LL))
   GDKY=ABS(DEY(LL)-DEY(LL))
   GDKZ=ABS(DEZ(LL)-DEZ(LL))
   CONXX=PXPX(NPT,LL)*WT
CONXY=PXY(NPT,LL)*WT
CONZZ=PZPZ(NPT,LL)*WT
IF(SSQ.EQ.0.0) GO TO 32
CONXX=CONXX+(PXPX(NBKPT,LL)-PXPX(NPT,LL))*WT/DIVNO
CONXY=CONXY+(PXY(NBKPT,LL)-PXY(NPT,LL))*WT/DIVNO
CONZZ=CONZZ+(PZPZ(NBKPT,LL)-PZPZ(NPT,LL))*WT/DIVNO
32 CONTINUE
83 FORMAT(1H ,3F12.5,2I10,2I15,F14.6,15)
GDKM=SORT(GDKX*GDKX+GDKY*GDKY+GDKZ*GDKZ)
IF(GDKM.LT.1E-05) GO TO 500
CALL CONDUC(SWXX,SWXY,SWZZ,SWJON,EN,NMAX)
GO TO 320
500 CONTINUE
CONTRIBUTION FROM CRITICAL POINTS ARE NEGLIGENCE
WRITE(6,84) GDKX,GDKY,GDKZ,NPT,KDX,KDY,KDZ,ENG,LG,LL,WT
84 FORMAT(1H ,3F12.5,2I10,2I15,F14.6,15)
320 CONTINUE
402 CONTINUE
401 CONTINUE
400 CONTINUE
IF(KX*KY*KZ.NE.KL/2-2.OR.NTEST.NF.0) GO TO 310
NTEST=1
KDZ=KZ*MAXBP+2
IF(KDZ.LT.0.OR.KDZ.GT.KLDIV) GO TO 310
KDY=KY*MAXBP+2
IF(KDY.LT.0.OR.KDY.GT.KLDIV) GO TO 310
KDX=KX*MAXBP+2
IF(KDX.LT.KDY.OR.KDX.GT.KLDIV) GO TO 310
SKZ=2.0*BDIV*2.0
SKX=SKZ
SKY=SKZ
GO TO 315
310 CONTINUE
REWIND 2
REWIND 1
311 CONTINUE
WRITE(6,45) SUMWT,VNORM,B,NMPT,NCRIT
45 FORMAT(1X,'SUM OF WEIGHT=',E12.5,5X,'VNORM=',F12.3,5X,'B=',F12.5,
      '5X,'NO OF POINT=',I8,5X,'NO OF CRT=',I5,1X)
RYTOW=13.6049*1.602191D-19*2.0*PI/6.626196D-34
CONST=3.10/D0/(PI*PI*274.074*5.2917D-9)
DO 701 NF=1,NMAX
CC=CONST/EN(NE)
SWXX(NE)=SWXX(NE)*CC
701 CONTINUE
SWXY(NE) = SWXY(NE) * CC
SWZZ(NE) = SWZZ(NE) * CC
EA = EN(NE)
EN(NE) = EN(NE) * 13.6049
WRITE(6, 702) EA, EN(NF), SWXX(NE), SWXY(NE), SWZZ(NE), SWJON(NE)
WRITE(7, 703) EN(NE), SWXX(NE), SWXY(NE), SWZZ(NE), SWJON(NE)
CONTINUE
701 FORMAT(2F7.3, 9(X, E10.4), 2F9.4)
702 FORMAT(5(E14.8, X1))
STOP
END
PROGRAM 12. COMPTON PROFILE.

REAL *8 (A-F,H-O-Z)
REAL *4 EUP(38), EDN(38)
DIMENSION KX(3000), KY(3000), KZ(3000)
DIMENSION UP(38), UP(38), GX(38,38)
DIMENSION KSOU(3000)
DIMENSION X(89), Y(89), Z(89)
DIMENSION ALS(14), ALD(5), COS(14), COP(11), COD(5), CS(4,14),
 & CP(3,11), CD(5,5)
COMMON/GTOCRYSTL, PI, ISATOM, IPATOM, IDATOM
COMMON/LCS/KSOU
COMMON/COMP/PX, PY, PZ, OMEGA, EXPVC, LSST, LSEND, LPST, LFEND, LST, LDEND
PI=3.14159265358979
51 FORMAT(2X,A8,3F10.5,815)
READ(5,51) CRYSTL, ACONST, FERMI, EXPVC, IDCUB, IBZDIV, NKPT, KSTOL,
 & KSINC, KSSTEP, K2MAX, INCIS
WRITE(6,52) ACONST, FERMI, IDCUB, IBZDIV, NKPT, K2MAX, KSTOL
OMEGA=ACONST**3/DFLOAT(IDCUB)
DIV=DFLOAT(IBZDIV)

DEFINE GAUSSIAN EXPONENTS AND EXPANSION COEFFICIENTS

4 FORMAT(815)
READ(5,4) ISOBNO, ISATOM, IP0BNO, IPATOM, IDOBNO, IDATOM
LSMAX=ISOBNO
LDMAX=IDOBNO
IF(ISATOM.NE.0) LSMAX=ISATOM
IF(IPATOM.NE.0) LDMAX=IDATOM
CALL RDGTO(ALS, ALD, COS, COP, COD, CS, CP, CD, ISOBNO, LMAX, IP0BNO,
 & LPMAX, IDOBNO, LDMAX, I)
LOST = 1
L0END = L0MAX * 5
LST = L0END + 1
LSEND = L0END + L0MAX
LPST = LSEND + 1
LPEND = LSEND + LPMAX * 3
PRINT 59
59 FORMAT (1H1)
C
C GENERATE PERMUTED RECIPROCAL LATTICE VECTORS
C
CALL GPERMK (KKX, KKY, KKZ, KSTOL, IDCUB, K2MAX, 1)
NCEND = LPEND
NCST = NCEND - 8
NBEND = NCST - 1
NBST = NBEND - 5
IF (INC15 .EQ. 0) NCEND = NCEND - 1
NB = LPEND
WRITE (6, 52) ACONST, FERMIE, IDCUB, IBZDIV, NKPT, K2MAX, KSTOL, L0MAX
& , ISOBN0, LPMAX, IPOBNO, L0MAX, IDORN0, EXPCVG, NBST, NBEND, NCST, NCEND
2, INC15
52 FORMAT (1X, 'LATTICE CONST=', F10.5, 2X, 'FERMI E=', F10.5, 2X, 'ATOMS/LAT'
1 TICE=', 15.2X, 'B.Z', 'DIV=', 15.2X, 'B.Z', 'PT=', 15.2X, 'MAX ', K**2=', 15.,
4, 2X, 'INCLUDE 1S=', 15.//)
62 FORMAT (15, 3F10.1)
ID100 = 100
ID110 = 110
ID111 = 111
AKR = 2.00 * PI / ACONST
CK = AKR / DIV
QROERR = CK * 0.001
C
C Q IS INVERSELY PROPORTIONAL TO THE CROSS SECTIONAL AREA OF EACH CJRE ON
C THE PLANE PERPENDICULAR TO & DIRECTION. & = X (1,0,0), & = N (1,1,0), & = L (1,1,1)
C
CONX = OMEGA**4.00 / (PI**2 * (ACONST / DIV)**2)
CONN = CONX / DSQRT (2.D0)
CONL = CONX * 0.7500 * DSQRT (3.00)
IF (IDCUB .NE. 1) CO = OFLT (IDCUB / 8.00)
IF (IDCUB .EQ. 1) CO = 1.00
TW = (2.00 * DIV)**3 * CO / 48.00
90 FORMAT (F10.5, 15)
C IN THE BRILLIQUIN ZONE.
C IF(IPUNCH.NE.0) RESULTS ARE PUNCHED.
C
IQ=0
91 CONTINUE
   READ(5,90,END=1000) Q,IPUNCH
   Q=Q*CK
   IQ=IQ+1
   COMPXV=0.00
   COMPXC=0.00
   COMPNC=0.00
   COMPNV=0.00
   COMPLC=0.00
   COMPLV=0.00
C SUM OVER R,L,V. IN SEVERAL STEPS TO CHECK CONVERGENCE.
C
KSST=1
   DO 900 KSJUM=1,KSSTEP
      KSEND=KSST+KSINC
      SUMW=0.00
      DO 100 KPT=1,NKPT
         C READ K, WEIGHT FACTORS, ENERGIES, AND WAVE FUNCTIONS NEGLECTING THE EFFECT
C OF SPIN-ORBIT COUPLING.
C
         READ(1) KX,KY,KZ,GT,(EUP(IJ),GX(JJ,II),JJ=1,NB),II=1,NB)
         DO 173 II=1,NB
            DO 173 JJ=1,NB
               XU(I,JJ)=GX(I,JJ)
            END
         END
         READ(2) KX,KY,KZ,GT,(EDN(I,JJ),GX(JJ,II),JJ=1,NB),II=1,NB)
         DO 174 II=1,NB
            DO 174 JJ=1,NB
               XD(I,JJ)=GX(I,JJ)
            END
         END
         XX(KPT)=DFLOAT(KX)*CK
         YX(KPT)=DFLOAT(KY)*CK
         ZX(KPT)=DFLOAT(KZ)*CK
         WT=GT
         SUMW=SUMW+WT
      END
   DO 200 KS=KSST,KSEND
      PX=XX(KPT)+AKR*XX(KS)
      PY=YX(KPT)+AKR*YX(KS)
      PZ=ZX(KPT)+AKR*ZX(KS)
C SELECT K POINTS THAT SATISFY THE MOMENTUM CONSERVATION RELATION.
c

ipx=0
if(dabs(px-q)*lt.qroerr) ipx=ipx+1
if(dabs(py-q)*lt.qroerr) ipx=ipx+1
if(dabs(pz-q)*lt.qroerr) ipx=ipx+1
if(dabs(px+q)*lt.qroerr) ipx=ipx+1
if(dabs(py+q)*lt.qroerr) ipx=ipx+1
if(dabs(pz+q)*lt.qroerr) ipx=ipx+1
ipn=0
if(dabs(q-px-py)*lt.qroerr) ipn=ipn+1
if(dabs(q-px+py)*lt.qroerr) ipn=ipn+1
if(dabs(q+px-py)*lt.qroerr) ipn=ipn+1
if(dabs(q+px+py)*lt.qroerr) ipn=ipn+1
if(dabs(q-py-pz)*lt.qroerr) ipn=ipn+1
if(dabs(q+py-pz)*lt.qroerr) ipn=ipn+1
if(dabs(q-py+pz)*lt.qroerr) ipn=ipn+1
if(dabs(q+py+pz)*lt.qroerr) ipn=ipn+1
if(dabs(q-pz-px)*lt.qroerr) ipn=ipn+1
if(dabs(q-pz+px)*lt.qroerr) ipn=ipn+1
ipl=0
if(dabs(q-px-py-pz)*lt.qroerr) ipl=ipl+1
if(dabs(q+px-py-pz)*lt.qroerr) ipl=ipl+1
if(dabs(q-px+py-pz)*lt.qroerr) ipl=ipl+1
if(dabs(q+px+py-pz)*lt.qroerr) ipl=ipl+1
if(dabs(q-py-px-pz)*lt.qroerr) ipl=ipl+1
if(dabs(q+py+px-pz)*lt.qroerr) ipl=ipl+1
if(dabs(q-py+px+pz)*lt.qroerr) ipl=ipl+1
if(dabs(q+py+px+pz)*lt.qroerr) ipl=ipl+1
if(ipx.eq.0. and ipn.eq.0. and ipl.eq.0.) go to 200

c
calculate the fourier transform of the localized basis function.
c
ccall fourfc(up,als,alp,ald,cs,cp,cd,lsmax,jpocko,
llmax,(do,nb),sumco)
sumco=0.0
do 103 ii=ncst,ncend
  ss=0.0
  tt=0.0
  do 202 jj=1,nb
    ss=ss+xup(jj,ii)*up(jj)
    tt=tt+xon(jj,ii)*up(jj)
  202 continue
  sumco=sumco+tt*tt+ss*ss
103 continue
901 CONTINUE
   IF (IPUNCH.EQ.0) GO TO 999
   WRITE(7,911) Q,PFX,PROFXC,PROFXV,ID10C
   WRITE(7,911) 0110,PFN,PROFN,PROFNY,ID110
   WRITE(7,911) 0111,PFL,PROFLC,PROFLV,ID111
   911 FORMAT(4E16.8,10X,16)
   999 CONTINUE
   GO TO 91
1000 CONTINUE
   IF (DABS(TW-SUMW).GT.0.1D-5) WRITE(6,5314) TW,SUMW
   5314 FORMAT(//,1X,*,SUMW=' ',2F10.6)
   STOP
   END
SUBROUTINE CONDUC(SWXX,SWXY,SWZZ,SWJON,EN,NEMAX)
C********************************************************************
C THE CONTRIBUTION OF EACH MINICELL TO THE CONDUCTIVITY TENSOR
C********************************************************************
DIMENSION SWXX(NEMAX),SWXY(NEMAX),SWZZ(NEMAX),EN(NEMAX),
1 SWJON(NEMAX)
COMMON/AR/ENG,GDKX,GDKY,GDKZ,GDKM,B2,B,CONXX,CONXY,CONZZ,CONST
ALX=GDKX/GDKM
ALY=GDKY/GDKM
ALZ=GDKZ/GDKM
C
NOW ARRANGE SUCH THAT ALX .GE. ALY , ALZ
C
IF(ALY .GE. ALZ) GO TO 351
ADD=ALY
ALY=ALZ
ALZ=ADD
351 IF(ALX .GE. ALY) GO TO 352
ADD=ALX
ALX=ALY
ALY=ADD
352 CONTINUE
W1=B*(ALX-ALY-ALZ)
W2=B*(ALX-ALY+ALZ)
W3=B*(ALX+ALY-ALZ)
W4=B*(ALX+ALY+ALZ)
AAXX=CONXX/GDKM
AAXY=CONXY/GDKM
AAZZ=CONZZ/GDKM
AAJON=CONST/GDKM
SMA=6.5*B2
DEMAX=(ALX+ALY+ALZ)*B*GDKM
DO 300 NF=1,NEMAX
EE=EN(NF)
C
MAX VALUE OF AREA CAN BE SQRT(3.)*4.*B*B=6.5*B*IF S,SMAX,ERROR POINTED
C
DEW=ABS(EE-ENG)
IF(DEW .GT. DEMAX) GO TO 300
W=DEW/GDKM
IF(W .GT. W4) GO TO 300
IF(W .GT. W1) GO TO 360
IF(ALX .GE. ALY+ALZ) GO TO 365
S=4.*B2/ALX
C
GO TO 395
S=((2.*((ALX*(ALY+ALZ)+ALY*ALZ)-1.)*B2-W**W)/(ALX*ALY*ALZ))
GO TO 395
360 CONTINUE
IF(W .GT. 2) GO TO 370
S=(B2*(ALX*(ALY+ALZ)+3.*ALY*ALZ)-B**W*(ALY+ALZ-ALX)-(W+W+B2/2.))/((ALX*ALY*ALZ))
GO TO 395
370 CONTINUE
IF(W .GT. W3) GO TO 375
S=2.*(B2*(ALX+ALY)-B**W)/(ALX*ALY)
GO TO 395
375 CONTINUE
S=((W4-W)**2)/(2.*ALX*ALY*ALZ)
GO TO 395
395 CONTINUE
IF(S .LT. SMAX) GO TO 899
WRITE(6,750)ALX,ALY,ALZ,W1,W2,W3,W4,W,S,NF,NPT
750 FORMAT(1H ,9E12.3,2I5)
899 CONTINUE
SWXX(NE)=SWXX(NE)+S*AAXX
SWXY(NE)=SWXY(NE)+S*AAXY
SWZZ(NE)=SWZZ(NE)+S*AAZZ
SWJON(NE)=SWJON(NE)+S*AAJON
300 CONTINUE
RETURN
END
SUBROUTINE COULOM(CHARGE, SUM, RS, FACT)
C*********************************************************************
C CALCULATE THE FOURIER COEFFICIENTS OF THE CHARGE DENSITY
C*********************************************************************
IMPLICIT REAL*8(A-F,H,O-Z)
DIMENSION CHARGE(1)
COMMON/CONST/A,RO,PI,ONFTHD
COMMON/VK0/C(7,11),EX(7,11),FACTO(10),IB(7,11),NDRB(7),NSTA
RS2=RS*RS
RS3=RS*RS2
CON=1.0
DO 79 I=1,NSTA
    DO 78 J=1,NN
        CD=C(I,J)*C(I,K)*C02*CON
        IA=IB(I,J)+IB(I,K)-1
        E=EX(I,J)+EX(I,K)
        EE=E*E
        T=EE*RS
        T2=T*T
        T27=(71,72,73,74,75,76,77),IAB
        SUM=SUM+2.0*E*CO/T2
    GO TO 78
72 SUM=SUM+2.0*CO*(3.0*EE-RS)/(T2*T)
    GO TO 78
73 SUM=SUM+24.0*E*CO*(EE-RS)/(T2*T2)
    GO TO 78
74 SUM=SUM+24.0*CO*(5.0*EE*EE-10.0*EE*RS+RS2)/(T**5)
    GO TO 78
75 SUM=SUM+24.0*CO*E*(3.0*EE*EE-10.0*EE*RS+3.0*RS2)/(T**6)
    GO TO 78
76 E4=EE*EE
    SUM=SUM+720.0*CO*(7.0*EE*E4-35.0*E4*RS+21.0*EE*RS2-8)*D0*EE*RS2-8*(T**7)
    GO TO 78
77 E4=EE*EE
    SUM=SUM+30.0*E*CO*(E4*EE-7.0*E4*RS+7.0*EE*RS2-8*(T**8)
78 CON=2.0
79 CON=1.0
RETURN
END
SUBROUTINE DENSIT(SWUP, SWDN, EN, NMAX)

C *****************************************************************
C CALCULATE THE CONTRIBUTION TO THE DENSITY OF STATES
C *****************************************************************

DIMENSION SWUP(NMAX), SWDN(NMAX), EN(NMAX)

COMMON/AR/ENG..GDKX..GDKY..GDKZ..GDKM..B2..B..CONUP..CONDN

ALX=GDKX/GDKM
ALY=GDKY/GDKM
ALZ=GDKZ/GDKM

C
NOW ARRANGE SUCH THAT ALX .GE. ALY .GE. ALZ

IF(ALY .GE. ALZ) GO TO 351

ADD=ALY
ALY=ALZ
ALZ=ADD

351 IF(ALX .GE. ALY) GO TO 352

ADD=ALX
ALX=ALY
ALY=ADD

IF(ALY .LT. ALZ) GO TO 353

352 CONTINUE

W1=B*ABS(ALX-ALY-ALZ)
W2=B*(ALX-ALY+ALZ)
W3=B*(ALX+ALY-ALZ)
W4=B*(ALX+ALY+ALZ)

AAUP=CONUP/GDKM
AADN=CONDN/GDKM

SMAX=6.5*B2
DEMAX=(ALX*ALY*ALZ)*B*GDKM

C

C CALCULATES AREA OF PLANE OF ENERGY *E* IN A GIVEN CUBE.
MAX VALUE OF AREA CAN BE SQRT(3)*4.*B*B=6.5*B*B, IF S, SMAX ERROR POINTED

DO 300 NE=1,NMAX

EE=EN(NE)

DEW=ABS(EE-ENG)

IF(DEW .GE. DEMAX) GO TO 300

W=DEW/GDKM

IF(W .GT. W4) GO TO 300

IF(W .GT. W1) GO TO 360

IF(ALX .LT. ALY+ALZ) GO TO 365

S=4.*B2/ALX

GO TO 395

365 S=((2.*(ALX*(ALY+ALZ)+ALY*ALZ)-1.)*B2-W*W)/(ALX*ALY*ALZ)

GO TO 395

360 CONTINUE

IF(W .GT. W2) GO TO 370


\[ S = \frac{B_2(\text{ALX}(\text{ALY}+\text{ALZ})+3*\text{ALY}\cdot\text{ALZ})-B*W(\text{ALY}+\text{ALZ}-\text{ALX})-(W*W+B_2)/2.))}{\text{ALX} \cdot \text{ALY} \cdot \text{ALZ}} \]

370 CONTINUE
   IF(W .GT. W3) GO TO 375
   S = 2.*(B2*(ALX+ALY)-B*W)/(ALX*ALY)
   GO TO 395
375 CONTINUE
   S = ((W4-W)**2)/(2.*ALX*ALY*ALZ)
395 CONTINUE
   IF(S .LT. SMAX) GO TO 899
WRITE(6,750)ALX,ALY,ALZ,W1,W2,W3,W4,W,S,NF,NPT
750 FORMAT(1H ,9E12.3,2I5)
899 CONTINUE
   SWUP(NE)=SWUP(NE)+S*AUP
   SWDN(NE)=SWDN(NE)+S*AADN
300 CONTINUE
RETURN
END
SUBROUTINE FOURFC(UP, ALS, ALP, ALD, CS, CP, CD, ISOBNO, LSMAX, IPOBNO,  
LPMAX, IDOBNO, LDMAX)
C*******************************************************************************
C CALCULATE THE FOURIER TRANSFORM OF THE LOCALIZED BASIS FUNCTION.
C*******************************************************************************
IMPLICIT REAL *8 (A-F,H,O-Z)
DIMENSION UP(1), ALS(1), ALP(1), ALD(1),
CS(LSMAX, ISOBNO), CP(LPMAX, IPOBNO), CD(LDMAX, IDOBNO)
COMMON/COMP/PX, PY, PZ, OMEGA, EXPCVG, LSST, LSEND, LPST, LPEND, LDST, LDEND
PI=3.141592653589793
DO 10 I=1, LPMAX
10 UP(I)=0.D0
CC=1.00/DSQRT(OMEGA)
PP=PX*PX+PY*PY+PZ*PZ
S-FUNCTIONS
DO 20 NS=1, ISOBNO
DEL=PP/(4.0*D0*ALS(NS))
IF (DEL.GT.EXPCVG) GO TO 20
DEL=DEXP(-DEL)
SLAM=PI/ALS(NS)
CONST=CC*SLAM*DSQRT(SLAM)*DEL
DO 21 IS=1, LSMAX
II=IS*LDEND
21 UP(II)=UP(II)+CONST*CS(IS, NS)
20 CONTINUE
P-FUNCTIONS
DO 30 NP=1, IPOBNO
DEL=PP/(4.0*D0*ALP(NP))
IF (DEL.GT.EXPCVG) GO TO 30
DEL=DEXP(-DEL)
SLAM=PI/ALP(NP)
CONST=-CC*SLAM*DSQRT(SLAM)*DEL/(2.0*ALP(NP))
DO 31 IP=1, LPMAX
PCO=CONST*CP(IP, NP)
II=3*(*IP-1)
IX=II*LSEND+1
IY=II*LSEND+2
IZ=II*LSEND+3
UP(IX)=UP(IX)+PCO*PX
UP(IY)=UP(IY)+PCO*PY
UP(IZ)=UP(IZ)+PCO*PZ
31 CONTINUE
D-FUNCTIONS

PXV = PX*PY
PYZ = PY*PZ
PZX = PZ*PX
PX2 = (PX*PX - PY*PY) / 2.0
PZ2 = (3.00*PZ*PZ - PP) / (2.00*DSQRT(3.00))

DO 40 ND = 1, ID0BN0
DEL = PP / (4.00*ALD(ND))
IF (DEL .GT. EXPCVG) GO TO 40
DEL = DEXP(-DEL)
SLAM = PI / ALD(ND)
CONST = CC*SLAM*DSQRT(SLAM)*DEL / (4.00*ALD(ND)*ALD(ND))

DO 41 ID = 1, LDMAX
DCO = CONST*CD(ID, ND)
NDXY = ID
NDYZ = NDXY + LDMAX
NDZX = NDYZ + LDMAX
NDX2 = NDZX + LDMAX
NDZ2 = NDX2 + LDMAX
UP(NDXY) = UP(NDXY) + DCO*PX
UP(NDYZ) = UP(NDYZ) + DCO*PYZ
UP(NDZX) = UP(NDZX) + DCO*PZX
UP(NDX2) = UP(NDX2) + DCO*PX2
UP(NDZ2) = UP(NDZ2) + DCO*PZ2

41 CONTINUE
40 CONTINUE
RETURN
END
SUBROUTINE FUNCT(M)

C***********************************************************************
C Y IS REPLACED BY (OV**-1) Y
C (KK,I,J)=2*M*(J-1)+2*(I-1)+KK
C (KK,N,J)=2*M*(J-1)+2*(N-1)+KK
C***********************************************************************
REAL*8 Y,OV
COMMON/B/Y(11552)
COMMON/C/OV(2926)
M2=M*2
DO 100 I=1,M
II=M+I-1
LL=II*(II+1)/2
II2=2*(II-1)
DO 100 J=1,M
DO 100 KK=1,2
JKK=M2*(J-1)+KK
KKIJ=JKK+II2
IF(II,EQ,M) GO TO 102
II=II+1
DO 101 N=11,M
IN=N*(N-1)/2+II
KKNJ=JKK+2*(N-1)
Y(KKIJ)=Y(KKIJ)-OV(IN)*Y(KKNJ)
101 CONTINUE
102 CONTINUE
Y(KKIJ)=Y(KKIJ)/OV(LL)
100 CONTINUE
RETURN
END
SUBROUTINE GBZPT(KBX,KBY,KBZ,WT,KPT,IDCUB,KBZPT,TW)
C***********************************************************************
C SC IDCUB=1, RRC IDCUB=2, FCC IDCUB=4
C WT=THE FRACTION OF EACH CUBE CENTERED AT EACH (KRX,KRY,KRZ) THAT LIES
C WITHIN THE INDEPENDENT 1/48TH OF THE B, Z.
C TW=SUMW=THE SUM OF WT IN THE 1/48TH OF THE ZONE
C KPT=TOTAL NO OF POINTS GENERATED
C***********************************************************************
REAL*8 W, SUMW, WT(1), TW
INTEGER*2 KBX(1), KBY(1), KBZ(1)
KPT=0
KL=KBZPT-1
SUMW=0.0
IF(IDCUB.NE.4) GO TO 110
DO 100 I=1,KBZPT
  DO 100 J=1,II
  DO 100 K=1,JJ
  KX=II-1
  KY=JJ-1
  KZ=KK-1
  KT=KX*KY*KZ
  KM=KL*3/2
  IF(KT.GT.KM) GO TO ICO
  KPT=KPT+1
  W=1.0
  IF(KT.EQ.KM) W=W*0.5DO
  IF(KX.EQ.KL) W=W*0.5DO
  IF(KX.EQ.0) W=W*0.5DO
  IF(KY.EQ.0) W=W*0.5DO
  IF(KZ.EQ.0) W=W*0.5DO
  IF((KX.EQ.KY.OR.KY.EQ.KZ)) W=W*0.5DO
  IF(KX.EQ.KZ) W=W/3.0
  KBX(KPT)=KX
  KBY(KPT)=KY
  KBZ(KPT)=KZ
  WT(KPT)=W
  WRITE(6,6) KPT,KX,KY,KZ,W
  SUMW=SUMW+W
100 CONTINUE
GO TO 310
110 IF(IDCUB.NE.2) GO TO 210
KPT=0
DO 200 I=1,KBZPT
  DO 200 J=1,II
  DO 200 K=1,JJ
  DO 200 II=1,II
  DO 200 JJ=1,II
  DO 200 KK=1,II
  DO 200 II=1,II
  DO 200 JJ=1,II
  DO 200 KK=1,II
299
KX=I I-1
KY=JJ-1
KZ=KK-1
KT=KX+KY+KZ
KM=KL*3/2
IF(KT.GT.KM) GO TO 200
KXY=KX+KY
IF(KXY.GT.KL) GO TO 200
KPT=KPT+1
W=1.D0
IF(KX.EQ.KL) W=W*0.5D0
IF(KY.EQ.KL) W=W*0.5D0
IF(KZ.EQ.KL) W=W*0.5D0
IF(KX.EQ.KY.OR.KY.EQ.KZ) W=W*0.5D0
IF(KX.EQ.KZ) W=W*0.5D0
KYZ=KY+KZ
IF(KXY.EQ.KL.AND.KYZ.EQ.KL.AND.KY.NE.KL/3) W=W/3.D0
KBX(KPT)=KX
KBY(KPT)=KY
KBZ(KPT)=KZ
WT(KPT)=W
SUMW=SUMW+W
200 CONTINUE
GO TO 310
210 IF(IDCUB.NE.1) STOP 3
KPT=0
DO 300 II=1,KBZPT
DO 300 JJ=1,II
DO 300 KK=1,JJ
KX=II-1
KY=JJ-1
KZ=KK-1
KPT=KPT+1
W=1.D0
IF(KX.EQ.KL) W=W*0.5D0
IF(KY.EQ.KL) W=W*0.5D0
IF(KZ.EQ.KL) W=W*0.5D0
IF(KX.EQ.KY.OR.KY.EQ.KZ) W=W*0.5D0
IF(KX.EQ.KZ) W=W*0.5D0
KBY(KPT)=KY
KBY(KPT)=KZ
KBZ(KPT)=KZ
\begin{verbatim}
WT(KPT)=
SUMW=SUMW+
300 CONTINUE
310 CONTINUE
   IF(IDCUB.NE.1) CO=DFLOAT(IDCUR)/8.0
   IF(IDCUB.EQ.1) CO=1.0
   TW=(2.00*DFLOAT(KL))^3*CO/48.0
   IF(TW.EQ.SUMW) RETURN
400 FORMAT(/,1X,'ATOMS/LATTICE=',3.5X,'SUM OF WT=',F12.6,/) WRITE(6,400) IDCUB,SUMW,TW RETURN
END
\end{verbatim}
SUBROUTINE GIINDPK(KKX,KKY,KKZ,KSQ,NKPT,IDCUB,K2MAX,NB,NSCAL,NPOPRT)
C**********************************************************************
C GENERATE INDEPENDENT RECIPROCAL LATTICE VECTORS WITH MAGNITUDE SQUARE LFSS
C THAN K2MAX
C IF(NPOPRT.NE.1) THE RECIPROCAL LATTICE VECTORS ARE SORTED IN ORDER OF
C INCREASING MAGNITUDE
C IF(NSCAL.NE.0) NO OF PERMUTATION FOR EACH VECTOR (NB) ARE GENERATED
C SC IDCUB=1, BCC IDCUB=2, FCC IDCUB=4
C**********************************************************************
INTEGER*2 KX(1),KY(1),KZ(1),NB(1),N
DIMENSION KSQ(1)
G=K2MAX
MAXKX=SQRT(G)*2
KPT=0
IF(IDCUB.NE.1) GO TO 200
DO 100 III=1,MAXKX,2
   DO 100 JJJ=1,III,2
      DO 100 KKK=1,JJJ,2
         KX=III-1
         KY=JJJ-1
         KZ=KKK-1
         DO 100 MMM=1,2
            K2=KX*KX+KY*KY+KZ*KZ
            IF(K2.GT.K2MAX) GO TO 101
            KPT=KPT+1
            IF(KPT.GT.NKPT) STOP 1
            IPT=KPT
            IF(KPT.EQ.1,OR,NPOPRT.EQ.0) GO TO 103
            IM=KPT-1
            IF(K2.GE.KSQ(IM)) GO TO 103
            IPT=KPT
102 KX(IPT)=KX(IM)
            KY(IPT)=KY(IM)
            KZ(IPT)=KZ(IM)
            KSQ(IPT)=KSQ(IM)
            III=III-1
            IM=IM-1
            IF(K2.LT.KSQ(IM)) GO TO 102
            IPT=III
103 KX(IPT)=KX
            KY(IPT)=KY
            KZ(IPT)=KZ
            KSQ(IPT)=K2
101 CONTINUE
KX=KX+1
KY=KY+1
200 CONTINUE
KZ=KZ+1
100 CONTINUE
GO TO 300
200 CONTINUE
DO 201 III=1,MAXXX
DO 201 JJJ=1,III
DO 201 KKK=1,JJJ
ITOL=III+JJJ+KKK-3
IF(ITOL.NE.(ITOL/2)*2,AND.IDCUB.EQ.2) GO TO 201
KX=III-1
KY=JJJ-1
KZ=KKK-1
K2=KX*KX+KY*KY+KZ*KZ
IF(K2.GT.K2MAX) GO TO 201
KPT=KPT+1
IF(KPT.GT.NKPT) STOP 1
IPT=KPT
IF(KPT.EQ.1,OR.ISORT.EQ.0) GO TO 203
IM=KPT-1
IF(K2.GE.KSQ(IM)) GO TO 203
II=KPT
202 KXX(II)=KXX(IM)
KKY(II)=KKY(IM)
KKZ(II)=KKZ(IM)
KSQ(II)=KSQ(IM)
IM=II-1
IF(K2.LT.KSQ(IM)) GO TO 202
IPT=II
203 KXX(IPT)=KX
KKY(IPT)=KY
KKZ(IPT)=KZ
KSQ(IPT)=K2
201 CONTINUE
300 CONTINUE
NKPT=KPT
IF(NBCAL.EQ.0) RETURN
DO 500 I=1,NKPT
KX=KXX(I)
KY=KKY(I)
KZ=KKZ(I)
N=48
IF(KX.EQ.0) N=N/2
IF(KY.EQ.0) N=N/2
IF(KZ.EQ.0) N=N/2
IF(KX.EQ.KY.OR.KY.EQ.KZ) N=N/2
GO TO 500
IF(KX.EQ.KZ) N=N/3
  NB(I)=N
  530 CONTINUE
  RETURN
END
SUBROUTINE GINTFC(FCS,NORD,NORDIM,NKDIM,NRDIM)
C******************************************************************************
C GENERATE FUNCTION G(N,K,R) DEFINED IN EQ. (2.44)
C******************************************************************************
IMPLICIT REAL *(A-F,H,O-Z)
DIMENSION FCS(NORDIM,NKDIM,NRDIM)
DIMENSION H(10),F(10)
COMMON/GFUC/AKR,*,DELW,DSTEP,MAXK,MAXR
NODD=(NORD/2)**2
IF(NOOD.EQ.NORD) NEVEN=NORD-1
IF(NOOD.NE.NORD) NEVEN=NORD
NODDM1=NODD-1
H(1)=1.0D0
RK=0.0D0
DO 200 K=1,MAXK
EXPA=-RK*RK*DELW
ADEL=DEXP(EXPA)
CONST=DELW*ADEL
IF(NEVEN.LT.3) GO TO 101
H(i)=RK*W
DO 100 N=3,NEVEN
NM1=N-1
NM2=N-2
H(N)=RK*W*H(NM1)-2.0D0*DFLOAT(NM2)*H(NM2)
100 CONTINUE
101 CONTINUE
RD=0.0D0
DO 205 NR=1,MAXR
C0K=RK*RK
C0=1.0D0
DO 201 L=1,NEVEN,2
FCS(L,K,NR)=CONST*H(L)*C0*DCOS(C0K)
C0=-C0*0.25D0
201 CONTINUE
RB=RD*DSTEP
205 CONTINUE
IF(NORD.EQ.1) GO TO 220
F(1)=ADEL
F(3)=(1.0D0-2.0D0/3.0D0*EXPA)*ADEL
IF(NOOD.LT.6) GO TO 202
DO 203 N=5,NODDM1,2
AN=DFLOAT(N)
F(N)=2.0D0*(AN+EXPA-1.5D0)*F(N-2)/AN-(1.0D0-3.0D0/AN)*F(N-4)
203 CONTINUE
202 CONTINUE
RD=0.0D0
DO 211 NR=1,MAXR
    CD0K=RD*RK
    CD0=1.D0
    DO 210 L=2,NOOD,2
        N=L-1
        CD0=CD0**DFLOAT(N)**0.5D0
        FCS(L,K,NR)=RK*F(N)*DELT*CD0*DSIN(CD0K)
    210 CONTINUE
    RD=RD+DSTEP
211 CONTINUE
220 RK=RK+AKR
200 CONTINUE
    N1=NOOD+2
    N2=NEVEN+2
    FINT=DELT
    DO 300 L=3,N2,2
300 FINT=FINT**DFLOAT(L-2)/2.D0
    DO 311 NR=1,MAXR
        FCS(N1,1,NR)=0.D0
311 FCS(N2,1,NR)=FINT
RETURN
END
SUBROUTINE GNBDE(DFK, DEKY, DEKZ, NKSUM, NB, NP, KLD, NKPT)
C*******************************************************************************
C       GENERATE ENERGY DERIVATIVES IN THE NEIGHBORING POINTS OF THE 1/16TH OF THE
C       BRILLOUIN ZONE
C       FOR C.C.C. LATTICE ONLY
C*******************************************************************************
INTEGER*2 NP(KLD,KLD,KLD)
DIMENSION DEKX(NKSUM,NB), DEKY(NKSUM,NB), DEKZ(NKSUM,NB)
NPT=NKPT
KL=KLD-2
KA=KL+1
KM=3*KL/2
DO 5 K=1,KA
DO 5 I=1,KA
DO 5 J=1,K
KT=I+J+K-3
IF(KT .NE. KM) GO TO 5
KXP=IABS(I-KL)
KYP=IABS(J-KL)
KZP=IABS(K-KL)
II=I+1
J1=J+1
K1=K+1
KXP1=KXP+1
KYP1=KYP+1
KZP1=KZP+1
KXP2=KXP+2
KYP2=KYP+2
KZP2=KZP+2
IF(I.GT.KL) GO TO 4
IF(K.GT.KL) GO TO 14
DO 20 NM=1,6
NPT=NPT+1
GO TO (21,22,23,24,25,26),NM
21 NP(I,J,K)=NPT
NOD=NP(KXP1,KYP2,KZP2)
IF(KXP1.GE.KYP2) GO TO 28
GO TO 29
22 NP(I,J1,K)=NPT
NOD=NP(KXP2,KYP1,KZP2)
IF(KXP2.GE.KYP1) GO TO 28
GO TO 29
23 NP(I,J,K1)=NPT
NOD=NP(KXP2,KYP2,KZP1)
IF(KXP2.GE.KYP2) GO TO 28
GO TO 29
24  NP(1, J, K) = NPT
   NOD = NP(KXP1, KYP1, KZP2)
   IF(KXP1.GE.KYP1) GO TO 28
   GO TO 29
25  NP(1, J, K1) = NPT
   NOD = NP(KXP1, KYP2, KZP1)
   IF(KXP1.GE.KYP2) GO TO 28
   GO TO 29
26  NP(1, J1, K1) = NPT
   NOD = NP(KXP2, KYP1, KZP1)
   IF(KXP2.GE.KYP1) GO TO 28
28  DO 30 L = 1, NB
   DEKX(NPT, L) = -DEKY(NOD, L)
   DEKY(NPT, L) = -DEKZ(NOD, L)
   DEKZ(NPT, L) = -DEKX(NOD, L)
   CONTINUE
30  CONTINUE
29  CONTINUE
   GO TO 5
4  CONTINUE
   DO 40 NM = 1, 3
   NPT = NPT + 1
   GO TO (41, 42, 43), NM
41  NP(1, J1, K) = NPT
   NOD = NP(KXP1, KYP1, KZP2)
   IF(KXP1.GE.KYP1) GO TO 48
   GO TO 49
42  NP(1, J1, K1) = NPT
   NOD = NP(KXP1, KYP2, KZP1)
   IF(KXP1.GE.KYP2) GO TO 48
   GO TO 49
43  NP(1, J1, K1) = NPT
   NOD = NP(KXP2, KYP1, KZP1)
   IF(KXP2.GE.KYP1) GO TO 48
45  DO 45 L = 1, NB
   DEKX(NPT, L) = -DEKY(NOD, L)
   DEKY(NPT, L) = -DEKX(NOD, L)
   DEKZ(NPT, L) = -DEKZ(NOD, L)
   CONTINUE
46  CONTINUE
48  DO 46 L = 1, NB
11 CONTINUE
DEKX(NP1.L)=DEKZ(NOD.L)
DEKX(NP1.L)=DEKX(NOD.L)
DEKX(NP1.L)=DEKX(NOD.L)

DO 11 L=1,NB
NOD=N(P.L+1)*X(NP.NL)
NOD=N(P.L+1)*X(NP.NL)
NOD=N(P.L+1)*X(NP.NL)

IP(K.PD.L)*KPD.L=00 TO 10
IF(K.PD.L)*KPD.L=00 TO 10
IF(K.PD.L)*KPD.L=00 TO 10

CONTINUE
55 CONTINUE
DEKX(NP1.L)=DEKZ(NOD.L)
DEKX(NP1.L)=DEKX(NOD.L)
DEKX(NP1.L)=DEKX(NOD.L)

DO 55 L=1,NB
NOD=N(P.L+1)*X(NP.NL)
NOD=N(P.L+1)*X(NP.NL)
NOD=N(P.L+1)*X(NP.NL)

IF(K.PD.L)*KPD.L=00 TO 58
IF(K.PD.L)*KPD.L=00 TO 58
IF(K.PD.L)*KPD.L=00 TO 58

CONTINUE
46 CONTINUE
DEKX(NP1.L)=DEKZ(NOD.L)
DEKX(NP1.L)=DEKX(NOD.L)
10 CONTINUE
   WRITE(6,99) NPT
99 FORMAT(110)
   RETURN
END
SUBROUTINE GN9PT(PXPX,PXPY,PZPZ,NKSUM,NB,NP,KLD,NKPT,LG)

CIZES THE PRODUCT OF MOMENTUM MATRICES IN THE NEIGHBORING POINTS OF
C 1/16TH OF THE INDEPENDENT B. Z.
C
INTEGER*2 NP(KLD,KLD,KLD)
DIMENSION PXPX(NKSUM,NB),PXPY(NKSUM,NB),PZPZ(NKSUM,NB)
NPT=NKPT+1
KLD=KLD-2
KA=KL+1
KM=3*KL/2
DO 5 K=1,KA
  DO 5 I=1,KA
    DO 5 J=1,I
      KT=I+J+K-3
      IF(KT .NE. KM ) GO TO 5
      KXP=IABS(I—KL)
      KYP=IABS(J-KL)
      KZP=IABS(K-KL)
      II=I+1
      JI=J+1
      K1=K+1
      KXP1=KXP+1
      KYP1=KYP+1
      KZP1=KZP+1
      KXP2=KXP+2
      KYP2=KYP+2
      KZP2=KZP+2
      IF(I ,GT, KL) GO TO 4
      IF(K,GT, KL) GO TO 14
      NP(II, J, K)=NP(KXP1,KYP2,KZP2)
      NP(I, JI, K)=NP(KXP2,KYP1,KZP2)
      NP(I, J, K1)=NP(KXP1,KYP2,KZP1)
      NP(I, J1, K)=NP(KXP2,KYP1,KZP2)
      NP(I1, J1, K)=NP(KXP1,KYP1,KZP1)
      NP(I1, J1, K1)=NP(KXP2,KYP1,KZP1)
      DO 28 NM=1,6
      GO TO (21,22,23,24,25,26),NM
  5 CONTINUE
    IF(KXP1.GE,KYP2) GO TO 28
    IF(KXP1,GE,KYP1) GO TO 28
      CONTINUE
      IF(KXP2,GE,KYP2) GO TO 28
      IF(KXP2,GE,KYP1) GO TO 28
    CONTINUE
    END

GO TO 28
NOD = NP(KXP2, KYP1, KZP2)
GO TO 29
23 CONTINUE
IF (KXP2 .GE. KYP2) GO TO 28
NP(I, J, K1) = NPT
NOD = NP(KXP2, KYP2, KZP2)
GO TO 29
24 CONTINUE
IF (KXP1 .GE. KYP1) GO TO 28
NP(I1, J1, K) = NPT
NOD = NP(KXP1, KYP1, KZP2)
GO TO 29
25 CONTINUE
IF (KXP1 .GE. KYP2) GO TO 28
NP(I1, J1, K1) = NPT
NOD = NP(KXP1, KYP2, KZP1)
GO TO 29
26 CONTINUE
IF (KXP2 .GE. KYP1) GO TO 28
NP(I1, J1, K1) = NPT
NOD = NP(KXP2, KYP1, KZP1)
29 DO 30 L = 1, LG
PXPX(NPT, L) = PXPX(NOD, L)
PXPY(NPT, L) = - PXPY(NOD, L)
PZPZ(NPT, L) = PZPZ(NOD, L)
30 CONTINUE
NPT = NPT + 1
28 CONTINUE
GO TO 5
4 CONTINUE
NP(I1, J1, K) = NP(KXP, KYP1, KZP2)
NP(I1, J1, K1) = NP(KXP, KYP2, KZP1)
NP(I1, J1, K1) = NP(KXP, KYP1, KZP1)
DO 48 NM = 1, 3
GO TO (41, 42, 43), NM
41 CONTINUE
IF (KXP .GE. KYP1) GO TO 48
NP(I1, J1, K) = NPT
NOD = NP(KXP, KYP1, KZP2)
GO TO 49
42 CONTINUE
IF (KXP .GE. KYP2) GO TO 48
NP(I1, J1, K1) = NPT
NOD = NP(KXP, KYP2, KZP2)
GO TO 49
43 CONTINUE
IF(KXP .GE.KYP1) GO TO 48
NP(I,J1,K1)=NPT
NOD=NP(KXP,KYP1,KZP1)
49 DO 45 L=1,LG
  PXPX(NPT,L)=PXPX(NOD,L)
  PXPY(NPT,L)=PXPY(NOD,L)
  PZPZ(NPT,L)=PZPZ(NOD,L)
45 CONTINUE
NPT=NPT+1
48 CONTINUE
GO TO 5
14 CONTINUE
NP(I,J1,K)=NP(KXP2,KYP1,KZP)
NP(I,J,K)=NP(KXP1,KYP2,KZP)
NP(I,J1,K)=NP(KXP1,KYP1,KZP)
DO 58 NM=1,3
  GO TO (51,52,53),NM
51 CONTINUE
IF(KXP2.GE.KYP1) GO TO 58
NP(I,J1,K)=NPT
NOD=NP(KXP2,KYP1,KZP)
GO TO 59
52 CONTINUE
IF(KXP1.GE.KYP2) GO TO 58
NP(I,J,K)=NPT
NOD=NP(KXP1,KYP2,KZP)
GO TO 59
53 CONTINUE
IF(KXP1.GE.KYP1) GO TO 58
NP(I,J1,K)=NPT
NOD=NP(KXP1,KYP1,KZP)
59 DO 55 L=1,LG
  PXPX(NPT,L)=PXPX(NOD,L)
  PXPY(NPT,L)=PXPY(NOD,L)
  PZPZ(NPT,L)=PZPZ(NOD,L)
55 CONTINUE
NPT=NPT+1
58 CONTINUE
CONTINUE
DO 10 I=1,KL
  DO 10 K=1,KA
  KT=I+I+J-3
  IF(KT.GT.KM) GO TO 10
  NP(I,I+1,K)=NPT
  NOD=NP(I+1,I,K)
10 DO 11 L=1,LG
PXPX(NPT, L) = PXPX(NOD, L)
PXPY(NPT, L) = -PXPY(NOD, L)
PZPZ(NPT, L) = PZPZ(NOD, L)

CONTINUE
NPT = NPT + 1
CONTINUE
WRITE(6, 99) NPT
FORMAT(110)
RETURN
END
SUBROUTINE GNOPUM(NPUM, NTYP, N, ND, NARTOL, NORDA, NORDB, NSYMP)

C ***********************************************************************
C NPUM DEFINES THE GROUP OPERATIONS THAT GENERATES THE STAR OF R
C NTYP DEFINES THE TERM IN THE EXPANSION OF EXP(I K.R) H(R) WHICH IS AN EVEN
C FUNCTION OF RX, RY, AND RZ.
C***********************************************************************

INTEGER*2 N(ND,ND,ND,ND,ND,ND),NPUM(NARTOL,6),NTYP(NARTOL)

NM=0
DO 201 IA3=1,NORDA
DO 201 IA2=1,NORDA
DO 201 IA1=1,NORDA
IAT=IA1+IA2+IA3-2
IF(IAT.NE.NORDA) GO TO 201
DO 202 IB3=1,NORDB
DO 202 IB2=1,NORDB
DO 202 IB1=1,NORDB
IBT=IB1+IB2+IB3-2
IF(IBT.NE.NORDB) GO TO 202
NM=NM+1
N(NA1,IA2,IA3,IB1,IB2,IB3)=NM
201 CONTINUE
202 CONTINUE

NM=0
DO 101 IA3=1,NORDA
DO 101 IA2=1,NORDA
DO 101 IA1=1,NORDA
IAT=IA1+IA2+IA3-2
IF(IAT.NE.NORDA) GO TO 101
DO 102 IB3=1,NORDB
DO 102 IB2=1,NORDB
DO 102 IB1=1,NORDB
IBT=IB1+IB2+IB3-2
IF(IBT.NE.NORDB) GO TO 102
NM=NM+1
NPUM(NM+1)=N(NA1,IA2,IA3,IB1,IB2,IB3)
NPUM(NM+2)=N(NA1,IA2,IA3,IB1,IB2,IB3)
NPUM(NM+3)=N(NA1,IA2,IA3,IB1,IB2,IB3)
NPUM(NM+4)=N(NA1,IA2,IA3,IB1,IB2,IB3)
NPUM(NM+5)=N(NA1,IA2,IA3,IB1,IB2,IB3)
NPUM(NM+6)=N(NA1,IA2,IA3,IB1,IB2,IB3)
IAB1=IA1+1
IAB2=IA2+1
IAB3=IA3+1
IF(NSYMP.EQ.0) GO TO 103
IAB1=IAB1+1
IAB2=IAB2+1

246
IAB3=IAB3+1

103 CONTINUE
   NT=1
   IF((IAB1/2)*2.NE.IAB1) NT=NT+1
   IF((IAB2/2)*2.NE.IAB2) NT=NT+2
   IF((IAB3/2)*2.NE.IAB3) NT=NT+4
   NTYP(NM)=NT
99 FORMAT(15,*,='(*,1X,3I1,*,*,3I1,1X,*'),3X,*NTYP=','15,1X,*PERMUTATION
1=('*,5(13,*,'),13,*'))
   WRITE(6,99) NM,IA1,IA2,IA3,IR1,IR2,IR3,NTYP(NM),(NPUM(NM,1),I=1,6)
102 CONTINUE
101 CONTINUE
RETURN
END
**SUBROUTINE** GPERMK(KX, KY, KZ, KSQ, NKPT, IDCUB, K2MAX, ISORT)

**C ******************************************************************************

**C**

**C** GENERATE PERMUTED RECIPROCAL LATTICE VECTORS WITH MAGNITUDE SQUARE LESS

**C** THAN K2MAX

**C** IF(ISORT.NE.0) THE RECIPROCAL LATTICE VECTORS ARE SORTED IN ORDER OF

**C** INCREASING MAGNITUDE

**C** SC IDCUB=1, BCC IDCUB=2, FCC IDCUB=4

**C ******************************************************************************

**C** INTEGER*2 KX(NKPT), KY(NKPT), KZ(NKPT)

**DIMENSION** KSQ(NKPT)

**G =K2MAX

**MAX=SQRT(G)+1**

**MAXX=2*MAX+1**

**KPT=0**

**IF(IDCUB.NE.4) GO TO 200**

**DO 100 III=1, MAXX, 2**

**DO 100 JJJ=1, MAXX, 2**

**DO 100 KKK=1, MAXX, 2**

**KX=III-1-MAX**

**KY=JJJ-1-MAX**

**KZ=KKK-1-MAX**

**DO 100 MMM=1, 2**

**K2=KX*KX+KY*KY+KZ*KZ**

**IF (K2.GT.K2MAX) GO TO 101**

**KPT=KPT+1**

**IF(KPT.GT.NKPT) STOP 2**

**IPT=KPT**

**IF(KPT.EQ.1.OR.ISORT.EQ.C) GO TO 103**

**IM=KPT-1**

**IF(K2.GE.KSQ(IM)) GO TO 103**

**II=KPT**

**102 KXX(II)=KXX(IM)**

**KKY(II)=KKY(IM)**

**KKZ(II)=KKZ(IM)**

**KSQ(II)=KSQ(IM)**

**II=II-1**

**IM=II-1**

**IF(II.GT.1.AND.K2.LT.KSQ(IM)) GO TO 102**

**IPT=II**

**103 KXX(IPT)=KX**

**KKY(IPT)=KY**

**KKZ(IPT)=KZ**

**KSQ(IPT)=K2**

**101 CONTINUE**

**KX=KX+1**

**KY=KY+1**
SUBROUTINE GWTGAS(N, Y, XR, WR)
C***************************************************************
C FINDS ZEROS OF LEGENDRE POLYNOMIAL OF ORDER N AND THE CORRESP.
C WEIGHT FACTORS FOR THE GAUSSIAN INTEGRATION USING THE DEFINITION
C W(I)=2/((DP(N,X)/DX)**2 * (1-X*X)) AT X=X(I) WHERE P(N,X)=0 AND
C DP(N,X)/DX = N*P(N-1,X)/(1-X*X).
C Y IS AN WORKING FUNCTION DIMENSIONFD N+1
C***************************************************************
IMPLICIT REAL*8 (A-H,O-Z)
DIMENSION Y(1), XR(1), WP(1)
NHALF=N/2
WC=2.DO/DFLOATIN*N>
NR=0
DX=2.DO/DFLOATIN
IF(N .EQ. 2*(N/2)) GO TO 100
C
C IF ORDER IS ODD, ONE OF THE ZEROS IS X=0
C
XR(1)=0.DO
CALL DLEPI(Y,0.DO,N)  
WR(I)=WC/(Y(N)**2)  
NR=1
100 CONTINUE
XOLD=0.1D-5
DO 200 1=1,NHALF
  CALL DLEPI(Y,XOLD,N)
  YOLD=Y(N+1)
  NR=NR+1
  XNEW=XOLD+DX
  CALL DLEPI(Y,XNEW,N)
  YNEW=Y(N+1)
  IF(DX .LT. 1.D-16 .OR. DABS(YNEW) .LT. 1.D-16) GO TO 130
  YSGN=YNEW/YOLD
  IF (YSGN .GT. 0.) GO TO 120
120 XOLD=XNEW
  YOLD=YNEW
  GO TO 110
200 CONTINUE
C
C CLOSE-IN ON THE ZERO -- SIGN OF THE POLYNOMIAL HAS CHANGED.
C
DX=DX/2.DO
GO TO 110
130 XOLD=XNEW
  YOLD=YNEW
  GO TO 110
XR(NR)=XNEW
WR(NR)=WC*(1.D0-XNEW**2)/(Y(N)**2)
XOLD=0.1D-5*XNEW
DX=2.0D0/DFLOAT(N)

C SINCE THE ZEROS ARE MORE CROWDED NEAR X=1, DECREASE THE STEP SIZE AS WE GET CLOSER TO THIS END.
C

IF(NR.GT.1) DX=(XR(NR)-XR(NR-1))/2.D0

200 CONTINUE
DO 249 I=1,NR
 II=NR+I
 XR(II)=XR(I)
 WR(II)=WR(I)
249 CONTINUE

DO 250 I=1,NR
 II=2*NR-I+1
 XR(I)=-XR(II)
 WR(I)=WR(II)
250 CONTINUE

999 RETURN
END
$SICO(4, 7) = -\cos(I_1, K_1) * \sin(I_3, K_2) * \sin(I_2, K_3)$

$SICO(5, 7) = -\cos(I_3, K_1) * \sin(I_2, K_2) * \sin(I_1, K_3)$

$SICO(6, 7) = -\cos(I_2, K_1) * \sin(I_1, K_2) * \sin(I_3, K_3)$

$SICO(1, 8) = -\sin(I_1, K_1) * \sin(I_2, K_2) * \sin(I_3, K_3)$

$SICO(2, 8) = -\sin(I_2, K_1) * \sin(I_3, K_2) * \sin(I_1, K_3)$

$SICO(3, 8) = -\sin(I_3, K_1) * \sin(I_1, K_2) * \sin(I_2, K_3)$

$SICO(4, 8) = -\sin(I_1, K_1) * \sin(I_3, K_2) * \sin(I_2, K_3)$

$SICO(5, 8) = -\sin(I_3, K_1) * \sin(I_2, K_2) * \sin(I_1, K_3)$

$SICO(6, 8) = -\sin(I_2, K_1) * \sin(I_1, K_2) * \sin(I_3, K_3)$

RETURN

END
SURROUNDC GS1JFC(FCS,RK,NORD,NORDM,NRDIM)
C******************************************************************************
C GENERATE FUNCTION G(N,RK,R) IN EQ(B,44) FOR A GIVEN VALUE OF RK
C******************************************************************************
IMPLICIT REAL *8 (A-F,H,O-Z)
DIMENSION FCS(NORDM,NRDIM)
DIMENSION H(10),F(10)
COMMON/GSIJFC/»,DELT,»O4,0STFP,M*x»
NOOD=(NORD/2)*2
IF(NOOD.EQ.NORD) NEVEN=NORD-1
IF(NOOD.NE.NORD) NEVEN=NORD
NOODM1=NOOD-1
H(1)=1.DO
EXPA=-RK*RK**04
ADEL=DEXP(EXPA)
CONST=DELT*ADEL
IF(NEVEN.LT.3) GO TO 101
H(2)=RK*W
DO 100 N=3,NEVEN
NM1=N-1
NM2=N-2
H(N)=RK*W*H(NM1)-2.DO*W*DFLOAT(NM2)*H(NM2)
100 CONTINUE
101 CONTINUE
RD=0.DO
DO 205 NR=1,MAXR
CODK=RD*RK
CO=1.DO
DO 201 L=1,NEVEN,2
FCS(L,NR)=CONST*H(L)*CO*DCOS(CODK)
CO=-CO*0.2500
201 CONTINUE
RD=RD+DSTEP
205 CONTINUE
IF(NORD.EQ.1) RETURN
F(1)=ADEL
F(3)=(1.DO+2.DO/3.DO*EXPA)*ADEL
IF(NOOD.LT.6) GO TO 202
DO 203 N=5,NOODM1,2
AN=DFLOAT(N)
F(N)=2.DO*(AN+EXPA-1.5DO)*F(N-2)/AN-(1.DO-3.DO/AN)*F(N-4)
203 CONTINUE
202 CONTINUE
RD=0.DO
DO 211 NR=1,MAXR
CODK=RD*RK
211 CONTINUE
CO=1.D0
DO 210 L=2,N00D+2
   N=L-1
   CD=CD**3*DFLOAT(N)*0.5D0
   FCS(L, NR) = RK*F(N)*DELT*CO*DSIN(CODK)
210 CONTINUE
RD=RD+DSTEP
211 CONTINUE
RETURN
END
SUBROUTINE HRIN(M)

C **********************************************************************
C T IS REPLACED BY T (OV**-1)
C (KK, I, J) = 2*M*(J-1) + 2*(I-1) + KK
C (KK, I, N) = 2*M*(N-1) + 2*(I-1) + KK
C **********************************************************************

REAL*8 T, OV
COMMON/A/T(11552)
COMMON/C/OV(2926)
M2 = M*2
DO 100 J = 1, M
   JJ = J*(J+1)/2
   MJ = M2*(J-1)
   DO 100 KK = 1, 2
   DO 100 I = 1, M
      IKK = 2*(I-1) + KK
      KKIJI = MJ + IKK
      IF(J .EQ. 1) GO TO 102
      JK = J-1
      DO 101 N = 1, JK
         NJ = J*(J-1)/2+N
         KKIN = M2*(N-1) + IKK
         T(KKIJI) = T(KKIJI) - T(KKIN) * OV(NJ)
   101 CONTINUE
   102 CONTINUE
      T(KKIJI) = T(KKIJI) / OV(JJ)
   100 CONTINUE
RETURN
END
SUBROUTINE READ(SSA, PSA, SDA, PPA, PDA, DDA, SSB, PSB, SDB, PPD, PDR, DDR,
1 IASS, IAPS, IASD, IAPP, IAPD, IADD, ISSDIM, IPSDIM, ISODIM, IPDDIM,
2 IPDDIM, IDDDIM, CS, CP, CO, LSMAX, ISOBO, LPBMA, IPQBO, LDMAX, IDOBO)
C**********************************************************************
C READ IN THE INTEGRALS GENERATED IN PROGRAM 2 OR 3.
C NCHO(I)=1 COULOMB, 2 PARAMAGNETIC EXCH, 3 UP EXCH, 4 DOWN EXCH, 5 KINETIC,
C 6 OVERLAP, 7 PX, 8 PY, 9 PZ, ION PARAMAGNETIC, 11H UP, 12H DOWN.
C**********************************************************************
REAL*8 ALPHA, CS(LSMAX, ISOBO), CP(LPMAX, IPQBO), CD(LDMAX, IDOBO),
GX(360), CO, CM
INTEGER*2 NRC, M1, M2, NSYM
DIMENSION SSA(IASS, ISSDIM), SSB(IASS, ISSDIM), PSA(IAPS, IPSDIM),
1 PSB(IAPS, IPSDIM), SDA(IASD, ISODIM), SDR(IASD, ISODIM),
2 PPA(IAPP, IPDDIM), PPD(IAPP, IPDDIM), PDA(IAPD, IPDDIM),
3 PDB(IAPD, IPDDIM), DDA(IADD, IDDDIM), DDR(IADD, IDDDIM)
DIMENSION AX(10)
COMMON/ OBN O/ ALPHA, NKIND, NTOL, NCHO(5), ISYM
DO 111 NRC=1, IASS
  NRC=1, ISSDIM
  SSA(NRC, IJ)=0.0
  IF(NTOL.GT.1) SSB(NRC, IJ)=0.0
111 CONTINUE
110 READ(11, END=200) NRC, M1, M2, NSYM, (AX(NM), NM=1, NKIND)
  IF(NRC.GT.1) NRC=1, IASS
  IF(NRC.GT.1) GO TO 110
  DO 103 N=1, NTOL
    NTYP=NCHO(N)
    IF(NTYP.EQ.NKIND) BX(N)=AX(NTYP)
    IF(NTYP.EQ.NKIND+1) BX(N)=AX(1)+ALPHA*AX(2)+AX(5)
    IF(NTYP.EQ.NKIND+2) BX(N)=AX(1)+ALPHA*AX(3)+AX(5)
    IF(NTYP.EQ.NKIND+3) BX(N)=AX(1)+ALPHA*AX(4)+AX(5)
103 CONTINUE
  NRC=1, LSMAX
104 CONTINUE
  NRC=1, LSMAX
103 CONTINUE
  NTOL=1
  IF(NTOL.GT.1) SSB(NRC, IJ)=SSB(NRC, IJ)+BX(2)*CN
104 CONTINUE
  GO TO 110
200 CONTINUE
  NRC=1, IAPS
200 CONTINUE
  NRC=1, IPSDIM
  PSA(NRC, IJ)=0.0
  IF(NTOL.GT.1) PSB(NRC, IJ)=0.0
211 CONTINUE
210 READ(12,END=300) NRC,M1,M2,NSYM,(AX(NM),NM=1,NKIND)
   IF(NRC.GT.IAPS) GO TO 210
   DO 203 N=1,NTOL
       NM=(N-1)*3+NSYM
       NTYP=NCHO(N)
       IF(NTYP.LE.NKIND) BX(NN)=AX(NTYP)
       IF(NTYP.EQ.NKIND+1) BX(NN)=AX(1)+ALPHA*AX(2)+AX(5)
       IF(NTYP.EQ.NKIND+2) BX(NN)=AX(1)+ALPHA*AX(3)+AX(5)
       IF(NTYP.EQ.NKIND+3) BX(NN)=AX(1)+ALPHA*AX(4)+AX(5)
       IF(ISYM.NE.0) BX(NN)=-BX(NN)
   203 CONTINUE
   IF(NSYM.LE.3) GO TO 210
       IJ=0
       DO 204 I1=1,LPMAX
           DO 204 I2=1,LSMAX
               CO=CP(I1,M1)*CS(I2,M2)
               DO 204 NM=1,3
                   J=IJ+1
                   PSA(NRC,IJ)+=BX(NM)*CO
                   IF(NTOL.GT.1) PSA(NRC,IJ)+=BX(NM+3)*CO
               204 CONTINUE
       GO TO 210
   300 CONTINUE
   DO 311 NRC=1,IASD
       DO 311 IJ=1,ISDDIM
           SDA(NRC,IJ)=0.DO
           IF(NTOL.GT.1) SDB(NRC,IJ)=0.DO
       311 CONTINUE
   READ(13,END=400) NRC,M1,M2,NSYM,(AX(NM),NM=1,NKIND)
   IF(NRC.GT.IASD) GO TO 310
   DO 303 N=1,NTOL
       NN=(N-1)*6+NSYM
       NTYP=NCHO(N)
       IF(NTYP.LE.NKIND) BX(NN)=AX(NTYP)
       IF(NTYP.EQ.NKIND+1) BX(NN)=AX(1)+ALPHA*AX(2)+AX(5)
       IF(NTYP.EQ.NKIND+2) BX(NN)=AX(1)+ALPHA*AX(3)+AX(5)
       IF(NTYP.EQ.NKIND+3) BX(NN)=AX(1)+ALPHA*AX(4)+AX(5)
   303 CONTINUE
   IF(NSYM.LE.6) GO TO 310
       IJ=0
       DO 304 I1=1,LSMAX
           DO 304 I2=1,LDMAX
               CO=CS(I1,M1)*CD(I2,M2)
               DO 304 NM=1,6
                   IJ=IJ+1
               304 CONTINUE
SDA(NRC, IJ) = SDA(NRC, IJ) + BX(NM) * CO
IF (NTOL .GT. 1) SDB(NRC, IJ) = SDA(NRC, IJ) + BX(NM + 6) * CO

304 CONTINUE
GO TO 310

400 CONTINUE
DO 411 NRC = 1, IAPP
DO 411 IJ = 1, IPDDIM
PPA(NRC, IJ) = 0.0 DO
IF (NTOL .GT. 1) PPB(NRC, IJ) = 0.0 DO
411 CONTINUE

410 READ (14, END = 500) NRC, M1, M2, NSYM, (AX(NM), NM = 1, NKIND)
IF (NRC .GT. IAPP) GO TO 410
DO 403 N = 1, NTOL
NN = (N - 1) * 9 + NSYM
NTYP = NCH(O(N))
IF (NTYP .LE. NKIND) BX(NN) = AX(NTYP)
IF (NTYP .EQ. NKIND + 1) RX(NN) = AX(1) + ALPHA * AX(2) + AX(5)
IF (NTYP .EQ. NKIND + 2) RX(NN) = AX(1) + ALPHA * AX(3) + AX(5)
IF (NTYP .EQ. NKIND + 3) RX(NN) = AX(1) + ALPHA * AX(4) + AX(5)
403 CONTINUE
IF (NSYM .LT. 9) GO TO 410

I = 0
DO 404 I1 = 1, LPMAX
DO 404 I2 = 1, I1
CO = CP(I1, M1) * CP(I2, M2)
CM = CP(I2, M1) * CP(I1, M2)
DO 405 L1 = 1, 3
DO 405 L2 = 1, 3
NM = (L1 - 1) * 3 + L2
IJ = IJ + 1
PPA(NRC, IJ) = PPA(NRC, IJ) + BX(NM) * CO
IF (NTOL .GT. 1) PPB(NRC, IJ) = PPB(NRC, IJ) + RX(NM + 9) * CO
IF (M1 .EQ. M2) GO TO 405
NM = (L2 - 1) * 3 + L1
PPA(NRC, IJ) = PPA(NRC, IJ) + BX(NM) * CM
IF (NTOL .GT. 1) PPB(NRC, IJ) = PPB(NRC, IJ) + BX(NM + 9) * CM
405 CONTINUE
404 CONTINUE
GO TO 410

500 CONTINUE
DO 511 NRC = 1, IAPD
DO 511 IJ = 1, IPDDIM
PDA(NRC, IJ) = 0.0 DO
IF (NTOL .GT. 1) PDB(NRC, IJ) = 0.0 DO
511 CONTINUE

510 READ (15, FND = 600) NRC, M1, M2, NSYM, (AX(NM), NM = 1, NKIND)


```
I1 = I1 + 1
ODA(NRC, IJ) = DDA(NRC, IJ) + BX(NM) * CD
IF (NTOL * GT * 1) DDB(NRC, IJ) = DDB(NRC, IJ) + BX(NM+36) * CD
IF (M1 .EQ. M2) GO TO 605
NM = (L2-1) * 6 + LI
DDA(NRC, IJ) = DDA(NRC, IJ) + RX(NM) * CM
IF (NTOL * GT * 1) DDB(NRC, IJ) = DDB(NRC, IJ) + RX(NM+36) * CM
605 CONTINUE
604 CONTINUE
   GO TO 610
700 CONTINUE
RETURN
END
```
SUBROUTINE RDGTO(ALS, ALP, ALD, CS, CP, CD, SCO, PCO, DCO, ISOBNO, LSMAX,
& IPOBNO, LPMAX, IDOBNO, LDMAX, ICOMB)

C*******************************************************************************
C  DEFINE GTO & = S, P, AND D.
C  ISATOM=GTO NUMBERS FOR & SYMMETRY
C  ISATOM=ATOMIC BASIS NUMBER =0 IF INDEPENDENT GTO IS EMPLOYED
C  GS=NORMALIZATION CONSTANTS. ADDITIONAL ANGULAR FACTOR IS NECESSARY
C  FOR K**2-Y**2 (0.5), AND 3*Z**2-R**2 (0.5/SQRT(3.C)).
C  &ALL=GAUSSIAN EXPONENTIAL PARAMETERS FOR & SYMMETRY
C &CO=EXPANSION COEFFICIENTS FOR THE ATOMIC &-GTO=DELTA FUNCTION IF ISATOM=0
C  IF(ICOMB.NE.0) &CO=&CO*CS
C*******************************************************************************

IMPLICIT REAL*8 (A-F, H-O-Z)

DIMENSION ALS(1), ALP(1), ALD(1), CS(1), CP(1), CD(1), SCO(LSMAX, ISOBNO)
& PCO(LPMAX, IPOBNO), DCO(LDMAX, IDOBNO)

COMMON/GTO/CRYSTL.PI, ISATOM, IPATOM, IDATOM
DATA GWTS, GWTP, GWTD/*S*, *P*, *D*/

DO 10 J=1, ISOBNO
   READ(5, 11) ALS(J), (SCO(L, J), L=1, ISATOM)
   AAA=2.00*(8.00*ALS(J)**3/PI)**.2500
   CS(J)=AAA/D2SQRT(2500)
   WRITE(6, 15) CRYSTL, J, ALS(J), CS(J), (L, GWTS, SCO(L, J), L=1, ISATOM)
10 CONTINUE

IF(ISATOM.GT.0) GO TO 24

DO 22 N=1, ISOBNO
   DO 23 J=1, ISOBNO
      SCO(N,J)=0.00
   23 SCO(N,N)=1.00
24 IF(ICOMB.NE.0) GO TO 21

DO 25 N=1, LSMAX
   DO 26 J=1, ISOBNO
      SCO(N,J)=SCO(N, J)*CS(J)
25 CONTINUE

DO 26 J=1, IPOBNO
   READ(5, 11) ALP(J), (PCO(L, J), L=1, IPATOM)
   AAA=D2SQRT(3.00/PI)**.2500
   CP(J)=AAA/D2SQRT(2500)
26 CONTINUE

DO 30 J=1, ICOMB
   WRITE(6, 15) CRYSTL, J, ALP(J), CP(J), (L, GWTP, PCO(L, J), L=1, IPATOM)
30 CONTINUE

DO 31 N=1, LPMAX
   DO 32 J=1, IPOBNO
      PCO(N,J)=PCO(N, J)*CP(J)
31 CONTINUE

DO 32 N=1, IPOBNO
   DO 33 J=1, IPOBNO
      PCO(N,J)=0.00
33 CONTINUE

DO 34 J=1, ICOMB
   IF(ICOMB.NE.0) GO TO 31

DO 35 N=1, LPMAX
   DO 36 J=1, IPOBNO
      PCO(N,J)=PCO(N, J)*CP(J)
35 CONTINUE

DO 36 N=1, IPOBNO
   DO 37 J=1, IPOBNO
      PCO(N,J)=0.00
37 CONTINUE

DO 38 J=1, ICOMB
   IF(ICOMB.NE.0) GO TO 31

DO 39 N=1, LPMAX
   DO 40 J=1, IPOBNO
      PCO(N,J)=PCO(N, J)*CP(J)
39 CONTINUE

DO 40 N=1, IPOBNO
   DO 41 J=1, IPOBNO
      PCO(N,J)=0.00
41 CONTINUE

DO 42 J=1, ICOMB
   IF(ICOMB.NE.0) GO TO 31

DO 43 N=1, LPMAX
   DO 44 J=1, IPOBNO
      PCO(N,J)=PCO(N, J)*CP(J)
43 CONTINUE

DO 44 N=1, IPOBNO
   DO 45 J=1, IPOBNO
      PCO(N,J)=0.00
45 CONTINUE

DO 46 J=1, ICOMB
   IF(ICOMB.NE.0) GO TO 31

DO 47 N=1, LPMAX
   DO 48 J=1, IPOBNO
      PCO(N,J)=PCO(N, J)*CP(J)
47 CONTINUE

DO 48 N=1, IPOBNO
   DO 49 J=1, IPOBNO
      PCO(N,J)=0.00
49 CONTINUE

DO 50 J=1, ICOMB
   IF(ICOMB.NE.0) GO TO 31

DO 51 N=1, LPMAX
   DO 52 J=1, IPOBNO
      PCO(N,J)=PCO(N, J)*CP(J)
51 CONTINUE

DO 52 N=1, IPOBNO
   DO 53 J=1, IPOBNO
      PCO(N,J)=0.00
53 CONTINUE

DO 54 J=1, ICOMB
   IF(ICOMB.NE.0) GO TO 31

END
CONTINUE
DO 13 J=1,IDOBNO
READ(5,11) ALD(J),(DCO(L,J),L=1,IDATOM)
AAA=15.DO/DSQRT(15.DO)*(ALD(J)**7/(2.DO*PI))**0.2500
CD(J)=AAA*DSQRT(15.DO/4.DO/PI)
   13 WRITE(6,15) CRYSN,J,ALD(J),CD(J),(L,GWTD,DCO(L,J),L=1,IDATOM)
   IF(IDATOM.GT.0) GO TO 44
   DO 42 N=1,IDOBNO
   DO 43 J=1,IDOBNO
   43 DCO(N,J)=0.DO
   DO 44 N=1,LDMAX
   DO 45 J=1,LDMAX
   45 DCO(N,J)=DCO(N,J)*CD(J)
   CONTINUE
   11 FORMAT(F8.5,4D16.8)
   15 FORMAT(I8,A8,I2,2X,*EXPO=*,F13.6,*X,*NORM=*,F16.8,4(I3,A1,*=*,F14,*8))
RETURN
END
SUBROUTINE RTINH(M)

C**********************************************************************
C T IS REPLACED BY ((OV**T)**-1) T
C
C (KK, I, J) = 2*M*(J-1) + 2*(I-1) + KK
C
C (KK, N, J) = 2*M*(J-1) + 2*(N-1) + KK
C**********************************************************************
REAL*8 T, OV
COMMON/A/T(11552)
COMMON/C/OV(2926)
M2=M**2
DO 100 I=1,M
I2=2*(I-1)
I1=I*(I+1)/2
DO 100 KK=1,2
DO 100 J=1,M
JKK=M2*(J-1)+KK
KKIJ=JKK+I2
IF(I.EQ.1) GO TO 102
IK=I-1
DO 101 N=1,IK
NI=I*(I-1)/2+N
KKNJ=JKK+2*(N-1)
T(KKIJ)=T(KKIJ)-OV(NI)*T(KKNJ)
101 CONTINUE
102 CONTINUE
103 CONTINUE
T(KKIJ)=T(KKIJ)/OV(II)
100 CONTINUE
RETURN
END
SUBROUTINE SEXCH(AX,AY,AZ,IDIM)
C******************************************************************************
C THIS SUBROUTINE CALCULATES THE ZEROTH ORDER TERM IN THE KURIC HARMONIC
C EXPANSION OF DENSITY
C (RX(I),RY(I),RZ(I)) ARE FOUR DIRECTIONS CHOSEN TO CALCULATE THE ANGULAR
C AVERAGE OF DENSITY
C C41(I), C61(I), AND C81(I) ARE KURIC HARMONICS WITH L= 4, 6, AND 8.
C******************************************************************************
IMPLICIT REAL*8(A-F,H-O-Z)
DIMENSION AX(IDIM),AY(IDIM),AZ(IDIM)
DIMENSION RX(4),RY(4),RZ(4),WT(4),C41(4),C61(4),C81(4)
COMMON/VKO/C(7,11),EX(7,11),FACT0(10),IB(7,11),NORB(7),NSTA
COMMON/EXCH/R(96),W(96),EXCH(96),EXUP(96),EXDN(96)
COMMON/CHARGE/CHARGE(7),CHAHUP(7),CHARN(7)
COMMON/CONST/A,RO,PI,ONETHD
2 FORMAT(12F6.3)
READ(5,2) (RX(I),RY(I),RZ(I),I=1,4)
C
C CALCULATE THE WEIGHT FACTOR ALONG EXCH DIRECTION
C
CONST=1.DO/(4.DO*PI)
SD4PI=DSQRT(CONST)
DO 3 I=1,4
PR=RX(I)*RX(I)+RY(I)*RY(I)+RZ(I)*RZ(I)
RA=DSQRT(PR)
RX(I)=RX(I)/RA
RY(I)=RY(I)/RA
RZ(I)=RZ(I)/RA
X2=RX(I)*RX(I)
Y2=RY(I)*RY(I)
Z2=RZ(I)*RZ(I)
X4=X2*X2
Y4=Y2*Y2
Z4=Z2*Z2
C41(1)=1.25DO*DSQRT(21.DO)*((X4+Y4+Z4-0.6DO)
C61(1)=231.DO*DSQRT(26.DO)/8.DO*(X2*Y2*Z2+C41(1))/22.DO-1.DO/105.DO
C81(1)=65.DO*DSQRT(561.DO)/16.DO*(X4*X4+Y4*Y4+Z4*Z4-28.DO*C61(1))/
55.DO-210.DO*C41(1)/143.DO-1.DO/6.DO)
C41(I)=C41(I)*SD4PI
C61(I)=C61(I)*SD4PI
C81(I)=C81(I)*SD4PI
3 CONTINUE
W1=(C41(2)*C61(3)-C41(3)*C61(2))*C81(4)+(C41(4)*C61(2)-
C41(2)*C61(4))*C81(3)+(C41(3)*C61(4)-C41(4)*C61(3))*C81(2)
W2=(C41(2)*C61(4)-C41(4)*C61(2))*C81(3)+(C41(3)*C61(4)-C41(4)*C61(3))*C81(1)+(C41(4)*C61(1)-
C41(1)*C61(4))*C81(2)}
C41(I)*C61(4))*C81(3)+(C41(I)*C61(3)-C41(3)*C61(I))*C81(4)
C21(I)*C61(4))*C81(2)+(C41(I)*C61(2)-C41(2)*C61(I))*C81(3)
C21(I)*C61(4))*C81(1)+(C41(I)*C61(1)-C41(1)*C61(I))*C81(2)
C21(I)*C61(3)+C41(I)*C61(3)-C41(3)*C61(I)*C81(1)

\[ W_2 = (C_{41}(1) * C_{61}(4) * C_{81}(3) + (C_{41}(1) * C_{61}(3) - C_{41}(3) * C_{61}(1)) * C_{81}(4) \]
\[ W_3 = (C_{41}(2) * C_{61}(4) - C_{41}(4) * C_{61}(2)) * C_{81}(1) + (C_{41}(4) * C_{61}(1) - C_{41}(1) * C_{61}(4)) * C_{81}(3) \]
\[ W_4 = (C_{41}(2) * C_{61}(3) - C_{41}(3) * C_{61}(2)) * C_{81}(1) + (C_{41}(3) * C_{61}(1) - C_{41}(1) * C_{61}(3)) * C_{81}(2) \]
\[ W_5 = W_1 + W_2 + W_3 + W_4 \]
\[ W_T(1) = W_1/W_T \]
\[ W_T(2) = W_2/W_T \]
\[ W_T(3) = W_3/W_T \]
\[ W_T(4) = W_4/W_T \]

DO 4 I=1,4
WRITE(6,5) RX(I),RY(I),RZ(I),WT(I),C41(I),C61(I),C81(I)
PRINT 6
5 FORMAT(1X,*A=('1,'3F10.5,*'),5X,*WT=',*F10.5,5X,*K41=',*F10.5,3X,*K61
6 FORMAT(1H )

CALCULATE THE DENSITY ALONG FOUR DIRECTIONS (RX(I),RY(I),RZ(I)) AND TAKE THE AVERAGE

233 FORMAT(1X,/,14X,*R*,9X,*WT*,9X,*DENSITY*,10X,*DENSITY DOWN*,7X,
*C DENSITY DOWN*,7X)
DO 200 KR=1,96
DEN=0.D0
DENSUP=0.D0
DENSUP=0.D0
DO 200 ND=1,4
X=R(KR)*RX(ND)
Y=R(KR)*RY(ND)
Z=R(KR)*RZ(ND)
DO 72 I=1,NSTA
SUM=0.D0
DO 10 JJ=1,IDIM
PSI=0.D0
RA=SQRT((AX(JJ)-X)**2+(AY(JJ)-Y)**2+(AZ(JJ)-Z)**2)
DO 20 J=1,N
EAX=RA*EX(I,J)
IF(EAX.GT.40.D0)GO TO 101
IBI=IB(I,J)-1
REX=C(I,J)*RA**IBI*DEXP(-EAX)
GO TO 20
101 REX=0.0
20 PSI=PSI+REX
10 SUM=SUM+PSI*PSI
65 DENS = DENS + SUM * CHARGE(I) * CONST * WT(ND)
DENSUP = DENSUP + SUM * CHARUP(I) * CONST * WT(ND)
DENSDN = DENSDN + SUM * CHARDN(I) * CONST * WT(ND)
72 CONTINUE
201 CONTINUE
WRITE(6,231) KR, R(KR), W(KR), DENS, DENSUP, DENSDN
231 FORMAT(1X, 15, 2F11.5, 6F18.8)
EXCH(KR) = DENS
EXUP(KR) = DENSUP
EXDN(KR) = DENSDN
277 CONTINUE
RETURN
END
SUBROUTINE SPLOTE(S,F,E,NEPTS,EMIN,DE,FERMIE,NEMAX)
C
C PLOT THE DENSITY OF STATES
C
DIMENSION S(NEMAX),F(NEMAX),E(NEMAX)
I=NEPTS
J=I+1
K=I+2
CALL PLOT(0.5,-11,-3)
CALL PLOT(0.02,-3)
F(J)=EMIN
F(K)=DE*(I-1)/10.0
FERMIE=(FERMIE-E(J))/E(K)
WRT=FERMIE-0.32
CALL PLOT(FERMIE,0.0,3)
CALL PLOT(FERMIE,7.0,2)
CALL SYMBOL(WRT,7.5,0.214,0.0,4)
CALL SCALE(F,8.0,1.1)
CALL AXIS(0.0,0.11ENERGY (RY),-11,10,0,0,E(J),E(K))
CALL AXIS(0.0,0.37DENSITY OF STATES (ELECTRONS/ATOM-RY),37.9,
590,0.0,F(J),F(K))
CALL SYMBOL(1.0,7.5,0.21,13MAJORITY SPIN,0.0,13)
CALL LINE(E,F,1.0,0.0)
CALL PLOT(15,-11,-3)
CALL PLOT(0.0,2,-3)
CONTINUE
CALL PLOT(15,-11,-3)
CALL PLOT(0.0,2,-3)
IF(NSPIN0.EQ.2) GO TO 152
CALL PLOT(FERMIE,0.0,3)
CALL PLOT(FERMIE,7.0,2)
CALL SYMBOL(WRT,7.5,0.214,0.0,4)
DO 153 II=1,1
S(II)=S(II)+F(II)
CALL SCALE(S,8.0,1.1)
CALL AXIS(0.0,0.11ENERGY (RY),-11,10,0,0,E(J),E(K))
CALL AXIS(0.0,0.37DENSITY OF STATES (ELECTRONS/ATOM-RY),37.9,
590,0.0,F(J),F(K))
152 CONTINUE
SUBROUTINE SVKO(VKO)

C**Calculation of the Coulomb potential at k=(0,0,0)**

C***

IMPLICIT REAL*8(A-F,H,O-Z)
COMMON/VKO/C(7,11),FX(7,11),FACTO(10),IB(7,11),NORB(7),NSTA
COMMON/CHARGE/CHARGE(7),CHARUP(7),CHARDN(7)
VKO=0.D0
DO 23 L=1,NST
SUM=0.D0
CON=1.D0
N=NORB(L)
DO 20 J=1,N
DO 21 K=J,N
COL=C(L,J)*C(L,K)*CON
JA=IB(L,J)+IB(L,K)+2
EX=EX(L,J)+EX(L,K)
IR=JA+1
SUM=SUM*FACTO(JA)*COL/(EX**IR)
21 CON=1.D0
20 CON=2.D0
23 VKO=VKO+SUM*CHARGE(L)
RETURN
END

270
SUBROUTINE WFCC16(KX, KY, KZ, KL, WT)

C******************************************************************************
C FOR EACH(KX,KY,KZ) CALCULATE THE PORTION OF THE CUBE THAT LIES INSIDE THE
C 1/16TH OF THE INDEPENDENT B. Z. (F. C. C.)
C******************************************************************************
KM=3*KL/2
WT=1.0
KT=KX*KY*KZ
IF(KT .EQ. KM) WT=WT*0.5
IF(KX .EQ. KL) WT=WT*0.5
IF(KY .EQ. KL) WT=WT*0.5
IF(KZ .EQ. KL) WT=WT*0.5
IF(KZ .EQ. 0) WT=WT*0.5
IF(KY .EQ. 0) WT=WT*0.5
IF(KX .EQ. 0) WT=WT*0.5
IF(KX .EQ. KY) WT=WT*0.5
RETURN
END
VITA

Ching-ping Shih Wang was born on February 16, 1947 in Shanghai, China. In 1949 she and her family moved to Taiwan, Republic of China. She graduated from Taipei First Girls' High School in 1965. She received the degree of Bachelor of Science in Physics from Tunghai University, Taichung, Taiwan, in 1969. In September 1969, she came to the United States for post-graduate studies and received the degree of Master of Science from Louisiana State University, Baton Rouge, Louisiana, in January 1971. She is now a candidate for the degree of Doctor of Philosophy in the Department of Physics and Astronomy at Louisiana State University.

She is a member of the American Physical Society and of the National Honor Society Phi-Kappa-Phi.
EXAMINATION AND THESIS REPORT

Candidate: WANG, Ching-Ping Shih

Major Field: Physics

Title of Thesis: Band Structure of Nickel: Spin Orbit Coupling, the Fermi Surface, and the Optical Conductivity

Approved:

[Signature]
Major Professor and Chairman

[Signature]
Dean of the Graduate School

EXAMINING COMMITTEE:

[Signatures]

Date of Examination:

June 24, 1974