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Electronic Structure of Iron.

Diola Bagayoko

Louisiana State University and Agricultural & Mechanical College

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ELECTRONIC STRUCTURE OF IRON

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

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August 1983
DEDICATION

As an expression of my gratitude for their love and support, I dedicate this dissertation to my mother, Nagnouma (kind mother) Keïta; my father, Djigui (the reliant) Bagayoko; my grandfather, Namory (the great leader) Keïta; my grandmother, Mariam Traore; my wife, Ella Kelley; and my son, Namory Djigui Bagayoko.

I extend this dedication to the memories of my ancestor, Professor "Cheik" Mohamed Bagayoko of the University of Timbuctu, whose hard work, intellectual accomplishments, and great human qualities are a continual source of inspiration for me. In doing so I am hereby presenting this dissertation to my sons and daughters, present and future, as an invitation to uphold the family tradition.
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ABSTRACT

A survey of previous theoretical and experimental works on iron in some Bravais lattices and at various temperature and pressures shows this 3d transition metal to exhibit a wealth of allotropic transformations and to possess, along with some of its alloys, peculiar magnetic properties in the face centered cubic (FCC) phase. We present an ab-initio self-consistent spin polarized band structure study of this metal in the body (BCC) and face centered cubic lattices at absolute zero and at various atomic volumes. Our calculations employed gaussian basis functions in a LCAO scheme and used the RSK local density potential. In contrast to previous attempts, the structural and atomic volume dependences of the electronic and magnetic states of iron are analysed using the fundamental parameters, band widths and exchange splittings, of the energy bands.

While the smooth variation of the magnetic moment in BCC iron with lattice spacings greater or equal to 4.8 a.u. is attributed to the atomic origin of magnetism in that structural phase, its drastic change in FCC iron between \( a = 6.5516 \) a.u. and 7.0 a.u. is ascribed to a transition from an itinerant picture to a localized one. This analysis sheds some light on the nature of magnetism in other metals like cobalt. The relevance of the above transition to the properties of FCC iron based alloys is illustrated. Applications of the numerically established local quadratic dependence of the charge and spin form factors on the lattice spacing are discussed.
CHAPTER 1
INTRODUCTION

The BCC phase of iron is known to be the most stable one in ordinary conditions of temperature and pressure. The Curie or critical temperature of this ferromagnet is 1043 K. The equilibrium lattice spacing at 0 K is around 5.4057 a.u. A quasi-exhaustive list of theoretical band structure calculations of iron (Fe) at the equilibrium lattice constant (slightly different for different calculations) is provided by Tawil and Callaway, Callaway and Wang, and recent reviews. Unlike the case of nickel, there is a general agreement between theory and experiment for BCC iron as far as band widths and exchange splittings are concerned. The experimental spin splitting obtained at P by Eastman et al., 1.5 electron volts (eV) compares to the 1.34 eV theoretical result of Callaway and Wang. This is a significant agreement as the theoretical splittings for FCC nickel are generally double that of the experimental ones. The majority (or up) spin sub-band width at P is reported to be 3 and 2.6 eV by photo-emission experiment and theory, respectively. Danan and coworkers measured the magnetic moment to be 2.12 Bohr magneton ($\mu_B$) while theory predicted 2.16 $\mu_B$. Eastman et al. discussed the Fermi surface of iron and found theory and experiment to support one another.

The industrial importance of iron partly explains the continual growth of the number of experimental works on this 3d metal at finite temperature and under hydrostatic pressure. Under the
above conditions iron undergoes several allotropic transformations\textsuperscript{11,14} and exhibit a variety of magnetic properties. Liu and Bassett\textsuperscript{14} presented an experimental temperature versus pressure (T-P) phase diagram\textsuperscript{15,16} of iron. This diagram, whose general features are reproduced in Figure 1, illustrates the regions of stability for the alpha (\(\alpha\)), epsilon (\(\epsilon\)), gamma (\(\gamma\)), and delta (\(\delta\)) iron. The respective crystal structures are the body centered cubic (BCC), the hexagonal close packed (HCP), the face centered cubic (FCC), and a BCC with magnetic disorder.

A major obstacle in the study of FCC iron, as intimated by Figure 1, is the difficulty there is to stabilize it at low temperature\textsuperscript{11,17}. Several conclusions relevant to FCC iron are drawn from knowledge of various iron based alloys\textsuperscript{11}. While there seems to be agreement on the paramagnetism of a high pressure HCP phase of iron, the question of magnetism in the FCC phase is yet to be totally settled. A high temperature FCC phase (i.e., \(T = 1320\) K) is known to display spatial ferromagnetic correlations\textsuperscript{17}. Conflicting views exist on the magnetic state of the FCC phase assuming that it could be prepared at low temperature, and/or under high pressures. Kaufman et al.\textsuperscript{11} discussed the Mossbauer effect, neutron diffraction experiments as well as susceptibility measurements for various FCC alloys containing iron. It was concluded that at low temperatures, FCC iron would be antiferromagnetic (AF) with a moment less than one Bohr magneton (\(\mu_B\)). Two extrapolated lattice constants are obtained\textsuperscript{11} for FCC iron at 25 degree celsius using the atomic separation versus solute concentration curves\textsuperscript{18} of iron based alloys. The curves for Fe-Pt, Fe-Pd, Fe-Ni alloys in which iron
atoms possess a high moment (2.8 \( \mu_B \)) lead to 6.878 a.u. while those for Fe-C, Fe-Mn, Fe-N give 6.727 a.u. This was considered as supporting Tauer and Weiss\(^{19} \) hypothesis of low moment low volume (\( \gamma_1 \)) and high moment and high volume (\( \gamma_2 \)) states of FCC iron. The issue of magnetic order in FCC Fe has been closely related to that of its alloys in general and of the invar alloys in particular\(^{20} \). These invar alloys are characterized, among other things\(^{21} \), by an almost zero, if not negative, expansion coefficient in certain temperature and solute concentration ranges.

In contrast to some of the above works where the properties of FCC iron are inferred from those of alloys, Wright\(^{22} \), Gradmann et al.\(^{23} \), and Keune et al.\(^{24} \) considered pure gamma iron films. Wright studied by electron spin resonance 30 angstroms thick gamma Fe films grown by electrodeposition on the (110) copper (Cu) single crystal face. He found these films to display ferromagnetism at room temperature. A moment of 1.1 \( \mu_B \) and a lattice spacing of 6.8027 were estimated. Gradmann et al. performed magnetization measurements on gamma Fe thin films grown on the (111) copper surface. They utilized an oscillation type magnetometer. For temperatures in the range 70-300 K a ferromagnetic ordering was observed in these films. Keune and coworkers carried out Mossbauer spectroscopy measurements on gamma Fe films. The films were grown on the (001) copper face and were reported to exhibit antiferromagnetism for temperatures between 2 and 295 K. These authors\(^{24} \), considering the two previous results\(^{22,23} \), suggested a dependence of the magnetic ordering on the film orientation.
Figure 1. Major features of the temperature versus pressure (T-P) experimental phase diagram of iron according to Liu and Basset. The full, dotted, and dashed curves are respectively from references 14, 15, and 16.
Gonser et al.\textsuperscript{25} presented Mossbaur spectra of coherent FCC iron precipitates in a Cu\textsubscript{69}Au\textsubscript{30} matrix. Contrary to the antiferromagnetic results of previous works on gamma Fe precipitates, as reviewed by Kaufman et al.\textsuperscript{11}, these authors found ferromagnetic ones. They made measurements at 4.2, 77, and 295 K. They estimated an iron atom separation of at least 5.0227 a.u. using Vegards Law. Antiferromagnetism and ferromagnetism were intimated to occur for atomic separations respectively below and above this value. A significant result is the observation of ferromagnetism in gamma Fe by the microscopic Mossbauer technique as opposed to the macroscopic ones used in references 22 and 23. Very recently Brown et al.\textsuperscript{17}, on the basis of their ferromagnetic results from neutron diffraction experiments on FCC iron at high temperatures, concluded that the low temperature FCC iron, if it could be stabilized, would be ferromagnetic.

Several other theoretical works on FCC iron exist in the literature\textsuperscript{26-32}. The APW band structure calculations of Wood\textsuperscript{26} were followed by those of Deegan\textsuperscript{27} who used the narrow band approximation to the Korringa-Kohn-Rostoker (KKR) or the Green function method. Dalton\textsuperscript{28} presented density of state curves for BCC and FCC iron along with other metals.

More recently Madsen et al.\textsuperscript{29}, and Poulsen and coworkers\textsuperscript{30} addressed, among other issues, the question of magnetic order in BCC and FCC iron for various lattice parameters. They employed a local density potential and the atomic sphere approximation (ASA) to the KKR method. Their results and procedure of calculation are reviewed by Andersen et al.\textsuperscript{31}. For Wigner-Seitz radii ($R_s$) between 2.66 and
2.85 Madsen et al. found the magnetic moment of an assumed FCC phase to be between 3 and 3.5 $\mu_B$. The moment drops rapidly below 1.5 $\mu_B$ around $R_s = 2.60$ and goes to zero at $R_s = 2.47$. Poulsen et al., unlike Madsen and coworkers, included the sp-d hybridization in all their calculations and found no moment for FCC iron for $R_s$ values less than 2.60.

Kubler\textsuperscript{32} considered antiferromagnetism which was not addressed by the authors just mentioned. He also utilized a local density potential to carry out self-consistent band structure calculations in an augmented spherical wave approximation\textsuperscript{33}. He studied non-magnetic ferro and antiferromagnetic orderings in BCC and FCC iron. From the total energy curves he found the stable magnetic order to be ferro and antiferromagnetic for BCC and FCC iron phases, respectively. A difficulty connected with the FCC phase consists in having its total energy lower than that of ferromagnetic BCC iron for the $R_s$ values considered. We shall discuss this subsequently. The moment of the ferromagnetic FCC phase was found to exhibit the sharp drop described above around $R_s = 2.63$ and goes to zero in the vicinity of $R_s = 2.55$ a.u.

Roy and Pettifor\textsuperscript{34} reported to have obtained the $\gamma_1$ and $\gamma_2$ states from Stoner theory\textsuperscript{35}. The ASA and local density calculations of these authors predicted both states to be ferromagnetic. The experimental T-P diagram of iron in Figure 1 has very recently been qualitatively reproduced by Hasegawa and Pettifor\textsuperscript{36}. Their calculations were based on the spin fluctuation theory of band magnetism\textsuperscript{37,38}. They found the magnetic contribution to the free energy to be the driving force in the phase transitions.
and questioned previous explanations\textsuperscript{11} which employed the two gamma states.

From this survey it appears that the magnetic state of FCC ($\gamma$) iron at low temperature is yet to be determined as there are experimental and theoretical results to support opposite views.

Our goal is to study the problem of the stability of the magnetic structures by means of ab-initio self consistent electronic band structures of ferromagnetic iron in BCC and FCC Bravais lattices for some $R_s$ values between 2 and 5. Paramagnetism is indirectly allowed for. A close analysis of first principle energy bands and related fundamental parameters, band widths and splittings, is intended to explain essential electronic and magnetic properties of iron in the above phases as the lattice constant changes. The structural dependence of magnetism in iron is not only of importance in its own right but also is expected to be relevant to a complete understanding of invar anomalies.

The second chapter of this dissertation is devoted to an outline of our method of band structure calculation, the choice of a potential and the formalism for the calculation of the total energy of a metal recently developed by this group. The contraction procedure and other computational details are described in chapter two. The analysis of the results follows in chapter three and four. The electronic structure of BCC and FCC Fe are presented in the former while the latter addresses the magnetic properties. The discussions in the last chapter include some suggestions for future investigations believed to be of relevance to the properties of transition ferromagnets and a summary.
A modern treatment of energy band theory for a metal generally amounts to solving the Kohn-Sham equations\textsuperscript{39} of density functional theory\textsuperscript{39,40,41}. Indeed, assuming a potential describing the many particle system is known\textsuperscript{39,42} there exist several methods of obtaining the energy levels. These band calculation procedures have been reviewed by Callaway\textsuperscript{43}.

In the first section of this chapter we shall outline the linear combination of atomic orbital (LCAO) version of the tight-binding\textsuperscript{44} method. Our choice of an effective one particle density functional potential is discussed in the second section. A new formalism for the calculation of the total energy of a metal is then covered in the last one.

A. The LCAO Method

Our aim is to solve the single particle Schrödinger equation:

\[
(-\nabla^2 + V_\sigma(\vec{r})) \psi_n(\vec{k}, \vec{r}) = E_n(\vec{k}) \psi_n(\vec{k}, \vec{r})
\]

where

\[
V_\sigma(\vec{r}) = -\sum_{\mu} \frac{2z}{\mu} \frac{2z}{|\vec{r} - \vec{\mu}|} + 2 \int \frac{\rho(\vec{r}')}{|\vec{r} - \vec{r}'|} d^3r' + V_{xc\sigma}(\vec{r})
\]
and

$$\psi_n(\hat{k}, \hat{r}) = e^{-i\hat{k} \cdot \hat{R}} \psi_n(\hat{k}, \hat{r} + \hat{R}_\mu), \quad (3)$$

satisfies Bloch theorem. The band index \(n\), the coordinate vector \(\hat{r}\),
and the position vector \(\hat{R}_\mu\) for lattice site \(\mu\) are defined as usual.
The potential \(V_\sigma(\hat{r})\) comprises coulomb terms and an exchange
correlation contribution \(V_{xc\sigma}(\hat{r})\) where \(\sigma\) indicates the spin. The
nuclear charge is \(Z\) and the units of energy are Rydbergs (Ry) with
\(\hbar = c = 1, e^2 = 2, m = 1/2\).

The tight-binding method consists in searching for solutions to
equation 1 by expanding the wave function \(\Psi_n(\hat{k}, \hat{r})\) in a finite set of
atomic like (i.e., localized) functions. When the radial parts of
these functions are taken to be those obtained for atoms the method
is referred to as the LCAO method. The term LCGO, for linear
combination of gaussian orbitals, is used if the above radial parts
are gaussians. The basis functions \(\phi_i(\hat{k}, \hat{r})\) satisfy

$$\phi_i(\hat{k}, \hat{r}) = N^{-1/2} \sum_\mu e^{-i\hat{k} \cdot \hat{R}} U_i(\hat{r} - \hat{R}_\mu), \quad (4)$$

with

$$U_i(\hat{r}) = R_{\ell_i}(r) K_{\ell_i}^{\ell_i}(\Theta, \psi), \quad (5)$$
in which \(K_{\ell_i}^{\ell_i}(\Theta, \psi)\) and \(R_{\ell_i}(r)\), respectively, contain the angular
and radial dependences. The orbital quantum number is \(\ell_i\) and \(m\) is
the magnetic quantum number when the \(K_{\ell_i}^{\ell_i}(\Theta, \psi)\) are taken to be
spherical harmonics. In general the choices of $R^{i r}_i$ are

$$R^{l - a r}_i = N_i r^l e^{-a_i r} \quad \text{or} \quad R^{l - a r}_i = N_i r^l e^{-a_i r^2} \tag{6}$$

where $N_i$ is a normalization constant. For treatment of cubic crystals the angular functions are often chosen to be cubic harmonics. The substitution of

$$\psi_n(k^r, \mathbf{r}) = \sum C_{ni}(k^r) \phi_i(k^r, \mathbf{r}) \tag{7}$$

into equation 1 leads to

$$\sum_{i, j} H_{ij}(k^r) C_{nj}(k^r) = E_n(k^r) \sum_{j} S_{ij}(k^r) C_{nj}(k^r) \tag{8}$$

where

$$H_{ij}(k^r) = \sum_{\mu} e^{-ik^r \cdot \mathbf{r}_\mu} <U_i(\mathbf{r} - \mathbf{R}_\mu)| -\nabla^2 + V_o(\mathbf{r})| U_j(\mathbf{r})> \tag{9}$$

and the overlap matrix elements are

$$S_{ij}(k^r) = \sum_{\mu} e^{-ik^r \cdot \mathbf{r}_\mu} <U_i(\mathbf{r} - \mathbf{R}_\mu)| U_j(\mathbf{r})> \tag{10}$$

The matrix equation 8 is solved for the eigenvalues $E_n(k^r)$ and the expansion coefficients $C_{ni}(k^r)$.

It appears from equation 8 that the mathematical foundation of the LCAO method is the Rayleigh-Ritz variational formalism. In the absence of orthogonality between the basis functions, as is the case
here, the overlap matrix elements, $S_{ij}(\mathbf{k})$, appear explicitly.

To construct the potential $V_\sigma(\mathbf{r})$ one needs the charge density $\rho(\mathbf{r})$ which is generally obtained only when the correct wave functions of the occupied states of the system are known. For this reason, the most recent applications of the LCAO method involved an iterative procedure. The reader is referred to Wang and Callaway\textsuperscript{45} for details on the iterations. A second major problem in energy band theory, besides finding a method of solution to equation 1, is the choice of an effective potential as we shall discuss in the following section.

B. The RSK Local Density Functional Potential

The Slater exchange potential, proportional to the $1/3$ power of the charge density, is a well known example of an effective, local and single particle exchange potential. Hohenberg and Kohn\textsuperscript{41} proved that the ground state energy of a many electron system is a unique functional of its ground state charge density. Based on this theorem, Kohn and Sham\textsuperscript{39} and Sham and Kohn\textsuperscript{40} derived the equations describing real systems like metals. This led to the constructions of various exchange-correlation potentials, referred to as density functional potentials, which differ in their estimations of the unknown exact exchange-correlation contribution to the unique functional. One of the most used form is due to Von-Barth and Hedin (VBH)\textsuperscript{42}, a more soundly based version of which has been presented by Rajagopal, Singhal and Kimball (RSK)\textsuperscript{46}. This RSK potential has been fitted to the VBH functional forms, but possesses slightly different parameters.
The exchange or exchange-correlation potentials to be discussed depend on the spin, $\sigma$. This leads to a splitting of equation 1 into two, one for each spin. For ferromagnetic systems this leads to differences between eigenvalues $E_{n+}(\mathbf{k})$ and $E_{n-}(\mathbf{k})$, i.e., the exchange splittings.

Following Von Barth and Hedin, the exchange-correlation potential is written:

\[ V_{\text{xc}}(\mathbf{r}) = \frac{\partial}{\partial \rho_\sigma(\mathbf{r})} \left[ \rho(\mathbf{r}) \rho_{\text{xc}}(\rho_+(\mathbf{r}), \rho_-(\mathbf{r})) \right] \]

where

\[ \rho(\mathbf{r}) = \rho_+(\mathbf{r}) + \rho_-(\mathbf{r}) \]

\[ \rho_{\text{xc}}(\rho_+(\mathbf{r}), \rho_-(\mathbf{r})) = e_x + e_c \]

with

\[ e_x = -3 \left( \frac{3}{4\pi} \right)^{1/3} \left( \frac{\rho_+(\mathbf{r})^{4/3} + \rho_-(\mathbf{r})^{3/4}}{\rho(\mathbf{r})} \right), \]

\[ e_c = e_c^{\text{p}} + (e_c^f - e_c^f) f(x). \]

For

\[ x_+ = \frac{\rho_+(\mathbf{r})}{\rho(\mathbf{r})}, \quad x_- = \frac{\rho_-(\mathbf{r})}{\rho(\mathbf{r})} \]

and $a_0 = 2^{-1/3}$ one has

\[ f(x) = \frac{1}{1-a_0} (x_+^{4/3} + x_-^{4/3} - a_0) \]
The quantities $e^c_c$ and $e^f_c$ are expressed in terms of four constant parameters:

\[ c^p = 0.0504, \quad r^p = 30, \quad c^f = 0.0254, \quad r^f = 75 \text{ for VBH potential while} \]

\[ c^p = 0.04612, \quad r^p = 39.7, \quad c^f = 0.02628, \quad r^f = 70.6 \text{ for RSK potential.} \]

The merits of local density potentials are discussed in several review articles. In particular, as discussed by Callaway, the VBH type potentials give quite reasonable values of the band widths for metals while a typical Hartree-Fock treatment yields widths which are double that of the experimental ones. The recent work on lithium demonstrated that the RSK potential correctly describe the limit behavior of this metal for lattice constant larger than normal. In contrast to some Hartree-Fock results, the energy levels of metallic lithium unambiguously go to the atomic ones for lattice constants larger than about 14 a.u.

As for possible limitation of a local density potential as compared to non-local ones, the very recent study by Wang is a case in point. Wang performed self-consistent band structure calculations for FCC nickel utilizing a non-local density functional potential. This potential comprises a non-local exchange part constructed according to Gunnarson et al. weighted density approximation scheme and a local correlation contribution. The resulting exchange correlation energy per particle, contrary to the case of local approximations, goes to $1/r$ at large distance. It therefore formally reproduces the correct behavior away from a point charge. However
the results of Wang calculations, as compared to those obtained with the local WBH potential have mixed behaviors. Indeed, while the observed decrease of the exchange splitting from 0.6 eV to 0.4 eV was desired, the somewhat increase obtained for the band width was not.

A generally shared contention at present is that non-local forms of density functional potentials have yet to prove themselves to be superior to the local ones in practical applications. Perdew and coworkers obtained some results in that direction for atoms and other systems but the case of metals is not yet resolved.

In a LCAO scheme and using any WBH type potential we shall derive in the next section a formalism for the calculation of the total energy of a metal.

C. Evaluation of the Total Energy of a Metal

Callaway et al. recently presented a formalism for the evaluation of the total energy of a metal in the framework of an LCGO band structure calculation. After expressing the kinetic energy in terms of eigenvalues $E_{n\sigma}(\mathbf{k})$ one can write the total energy of a solid as:

$$\sum_{n=1}^{N} E_{n\sigma}(\mathbf{k}) = \sum_{\nu} \frac{\rho(\mathbf{r}) \rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \, d^3 r \, d^3 r' + \sum_{\mathbf{k}} \frac{Z_{\mu} Z_{\nu}}{|\mathbf{k} - \mathbf{\mathbf{k}}'_{\nu}|}$$

$$+ E_{xc} - \sum_{\sigma} \int \rho_{\sigma}(\mathbf{r}) \, V_{xc\sigma}(\mathbf{r}) \, d^3 r;$$

where the sum over $n$ and $\sigma$ is limited to occupied states. For a single species system as metallic lithium $Z_{\mu} = Z_{\nu} = Z$, the nuclear charge. The explicit exchange-correlation terms in equation 18 are
combined into $\Delta_{xc}$.

$$\Delta_{xc} = - E_{xc} + \frac{1}{2} \sum \rho_{\sigma}(\vec{r}) \nu_{xc\sigma}(\vec{r}) \ d^3r = \sum \rho_{\sigma}(\vec{r}) \ W_{\sigma}(\vec{r}) \ d^3r \quad (19)$$

where

$$W_{\sigma}(\vec{r}) = \rho(\vec{r}) \ \frac{\partial e_{xc}(\rho_+(\vec{r}), \rho_-(\vec{r}))}{\partial \rho_\sigma(\vec{r})} \quad (20)$$

It is to be noted that $E_{xc}$ is the exchange correlation contribution to the total energy not $\Delta_{xc}$. A major difficulty overcome by this group is that of evaluating the infinite Coulomb terms. These terms have been rearranged so as to obtain finite quantities $U$ and $D$ by setting

$$U + D = - \int \rho(\vec{r}) \ \rho(\vec{r}') \ \frac{d^3r \ d^3r'}{|\vec{r} - \vec{r}'|} + \sum_{\mu \neq \nu} \frac{Z_{\mu} Z_{\nu}}{|\vec{R}_{\mu} - \vec{R}_{\nu}|}$$

with

$$U = \sum_{\nu} Z_{\nu} \int \rho(\vec{r}) \ \frac{d^3r}{|\vec{r} - \vec{R}_{\nu}|} - \int \rho(\vec{r}) \ \rho(\vec{r}') \ \frac{d^3r \ d^3r'}{|\vec{r} - \vec{r}'|} \quad (21)$$

and

$$D = \sum_{\mu \neq \nu} \frac{Z_{\mu} Z_{\nu}}{|\vec{R}_{\mu} - \vec{R}_{\nu}|} - \xi Z_{\nu} \int \rho(\vec{r}) \ \frac{d^3r}{|\vec{r} - \vec{R}_{\nu}|} \quad (22)$$

For reasons to become clear in the following chapter, $U$ and $D$ are evaluated in reciprocal space.

$$U = - \frac{1}{2} \ N \ \Omega \ \sum_{s} \ V_{T}(\vec{R}_{s}) \ \rho_{p}(\vec{R}_{s}) \quad (23)$$
\[ D = \frac{1}{2} N Z\left[ (-\frac{Z}{2}) C - V_T(0) - \sum_{k h} V_e(k S) \right]. \quad (24) \]

In these expressions, restricted to a monotomic system, \( \Omega \) is the cell volume and the index \( e \) denotes the electronic contribution. \( V_T(K_s) \) is the Fourier transform of the total Coulomb potential, including the nuclear-nuclear repulsion, and \( K_s \) is a reciprocal lattice vector. \( V_T(0) \) is described by Callaway and the constant \( C \):

\[ C = \left( \frac{8\pi^3}{\Omega} \right) \sum_{k h} \frac{1}{K_s^2} - \int \frac{1}{q^2} d^3q, \quad (25) \]

has been evaluated by Pack et al. for various lattice structures. Following these authors' approach, this constant has been reevaluated to more significant figures in the course of the work on lithium. Boettcher went farther and found, in units of \( \frac{2\pi}{a} \):

\[
\begin{align*}
C &= -8.913632917586 \text{ for simple cubic lattice} \\
C &= -11.432989069675 \text{ for body centered cubic} \\
C &= -14.403769009759 \text{ for face centered cubic.}
\end{align*}
\]

The calculation of \( \Delta_{XC} \) is basically that of \( W_o(r) \) which, after some algebra, can be written

\[ W_o(r) = \left( \frac{1}{4} \mu_p^p + v_c + G \right) (2 x_o)^{1/3} + Q - G \quad (27) \]

with
\[ Q = \mu_c^p - \varepsilon_c^p - \nu_c, \quad G = \frac{a_o}{1-a_o} [\mu^F_c - \nu_c^F - \frac{7}{3} (\varepsilon_c^F - \varepsilon_c^D)] \]

The parameters in the expressions of \( W \) are as defined in reference 42 and \( a_o = 2^{-1/3} \).

The total energy is thus obtained as:

\[ N E_T = \sum_{k,\sigma} E_{n\sigma} (\vec{k}) + U + D - \Delta_{xc}. \quad (28) \]

Wang and Callaway\(^{45}\) implemented the LGCO method of band structure calculation using Slater type or WBH potentials. The resulting program package, BNDPKG, has been extended to evaluate the total energy \(49,50\). This program package has been used in the present study of iron, and the following chapter is devoted to the salient features of the computations.
CHAPTER 3
COMPUTATIONAL PROCEDURE

By computational procedure, what is meant here is the set of numerical techniques and details pertaining to the implementation of the formalisms in the preceding chapter. The major steps of the calculation are described, followed in the second section by the discussion of the contractions of basis sets.

A. BNDPKG

In a single particle approximation the band package, BNDPKG, produces the energy bands of a cubic material with one atom per unit cell. The calculations are non-relativistic and at absolute zero temperature. Para- or ferromagnetic orderings are allowed for and the LCGO method is chosen. The angular functions are cubic harmonics. The eigenvalues and wave functions are obtained at as many number of \( k \) points in \( 1/48^{th} \) of the first Brillouin zone as desired or economically feasible. Emphasis, in what follows, will be put on general features and new ones pertaining to the evaluation of the total energy. For further details we refer to Wang and Callaway\(^{45} \) and appendix A where some extended programs are provided.

FCOF is the first program of the package. It employs gaussians orbitals provided by atomic calculations to construct an initial charge density and then generates the fourier coefficients of the various terms in the potential, i.e., the electronic and total Coulomb and exchange-correlation potentials. The innocent looking
matrix elements, $H_{1j}(\hat{r})$, contain three dimensional multi-center integrals. As shown by Lafon and Lin\(^{58}\), the use of Fourier expansion, i.e.

$$V_{\sigma}(\hat{r}) = \int_0^\infty V_{\sigma}(\hat{r}_s) \cos \hat{r}_s \cdot \hat{r},$$

reduces the difficulties in the evaluation to at most two-center integrals. In the above expressions, the use of the cosine function is justified by the inversion symmetry of the potentials. The resulting two center integrals can be evaluated analytically if gaussian functions are used\(^{59,60,61}\).

An Ewald split technique is used to remedy a possible slow convergence of Fourier sums due to the screening potential of tightly bound electrons and the contribution of the nuclear terms. The choice of an effective exchange-correlation potential is determined by the input to subroutine VXCRS. Slater or VBH type potentials are currently allowed for. The new version of FCOF produces the Fourier coefficients of $W_{\sigma}(\hat{r})$ needed for the total energy calculation and contains a new approach to the computation of $V_T(0)$. This quantity has little bearing on the relative position of the energy levels but strongly affects the total energy as can be seen from equations 24 and 28.

Program ESINT evaluates integrals needed in the Hamiltonian and overlaps matrices and BND forms, using properties of the cubic group, the appropriate combinations to generate the matrix elements. In the event where self-consistency is not needed, the diagonalization option in BND is chosen to obtain the energies and wave functions.
We recall that only \( \mathbf{k} \)-points in the irreducible wedge (1/48\(^{th}\) of the first Brillouin zone) need be considered for cubic crystals. For self-consistency procedure the necessary Fourier transforms of the overlap integrals are generated and properly arranged in the fourth (SIJ) and fifth (INVS1J) programs respectively.

The iterations toward self consistency are performed in SCF1 and SCF2 for paramagnetic and ferromagnetic calculations respectively. Changes to the Fourier coefficients of the charge density, Coulomb and exchange-correlations potentials, are obtained and added to the appropriate quantities. Self-consistency is assumed to be reached when the Fourier coefficients of the Coulomb potentials from two consecutive iterations differ by no more than \( 10^{-4} \) for any \( \mathbf{k} \) vector. A judicious choice of the damping parameter FACT (i.e., 0.2 - 0.4) reduces the number of necessary iterations. SCF1 AND SCF2 has been extended to obtain the self-consistent Fourier transforms of \( W \) or \( W_\sigma \) respectively. The new version of SCF2 play a key role in the forthcoming discussion of the magnetic properties of iron.

Indeed, in the course of the study of metallic lithium\(^{49,50}\) the total energy of this material was computed using both para- and ferromagnetic inputs. For lattice constants less than 10.5 a.u. the paramagnetic calculations yielded energy bands identical to the up and down spin sub-bands of the ferromagnetic results and the two total energies agreed to over 5 decimal places. On the contrary, for lattice parameters above 10.7 a.u., lithium was found to be ferromagnetic. In this range the total energies for the ferromagnetic calculations were clearly lower than those resulting from the paramagnetic ones\(^{50}\). These results did not depend on the
input magnetic moment which was chosen between 0 and 1. Similar results have been obtained for copper. The important point here is that ferromagnetic calculations for iron, at various atomic volumes, are expected to yield a paramagnetic result if indeed iron is paramagnetic at the lattice constants considered.

The self-consistent results are fed into ESINT which outputs are used by BND to calculate the final self-consistent band structure. The last program of the package, DENST, generates the electronic density of states. This program has been extensively modified to evaluate the total energy expression in equation 28.

Bagayoko et al. used BNDPKG to obtain the electronic energies and other quantities for FCC copper at a lattice constant $a = 6.80915$ a.u. A basis set of 75 gaussian functions has been used and it took 417 CPU minutes (on an IBM 3033) to obtain self-consistent eigenvalues at 505 $k$ points of the irreducible wedge. The computations employed a paramagnetic input. Similar calculations with ferromagnetic inputs take about twice as much time. This makes it financially intractable to study BCC and FCC iron, with ferromagnetic inputs, at several lattice constants unless a method is found to significantly reduce the time needed. The contraction of the basis set is one such procedure as is discussed in the next section.

B. Contractions

Despite its advantages, i.e. analytical evaluation of integrals, the use of gaussian $(r^l e^{-\alpha r^2})$ basis sets has a drawback. Namely, the size of the Hamiltonian matrix is about twice as much as it would
be with exponential basis functions $r^\lambda e^{-\alpha r}$. Contraction
schemes has been developed $^{63-69}$ in order to reduce the dimension $N_d$
of the Hamiltonian matrices for atomic and molecular calculations.
Two methods generally utilized are the least square fit$^{66,68}$ and the
formation of linear combinations with fixed coefficients, of single
Gaussian type orbital (GTO)$^{63,65,69}$. The basis functions resulting
from the latter will be referred to as contracted Gaussian type
orbitals (CGTO), not to be confused with Gaussian type orbitals
obtained through a scaling of the exponents$^{70}$. Bagayoko$^{71}$ presented
guidelines for the construction of CGTO suitable for solid state
computations. Those are only surveyed here as further details are
available in reference 71.

The sets of GTO or CGTO provided for atoms are generally not
sufficient for molecular or solid state calculations. A major reason
for this is the difference between the electronic distributions in
atoms, molecules and solids. While the bond formation characterizes
molecules$^{69}$, the quasi-free electron behavior distinguish metals from
the latters and from atoms. One solution to the above inadequacy of
atomic GTO basis is the inclusion of supplementary orbitals$^{72,73}$. In
particular the atomic GTO must be supplemented by a 4p orbital in
order to correctly reproduce the electronic energy bands of 3d metals
around the fermi energy. A specific example is the disappearance of
copper fermi surface neck at L, as shown by Bagayoko$^{73}$, if a 4p like
orbital is not used. Another, relatively minor, modification of the
atomic GTO sets is the dropping of the atomic s orbital with the
smallest exponent for calculations on 3d metals.

The similarity of the core electronic cloud in atoms, molecules,
and solid supplemented by the fact that the largest number of orbitals, for a given symmetry (s, p, d, or f), contribute to the innermost atomic functions lead to an obvious first rule to follow in forming CGTO. It consists in grouping orbitals with consecutive exponents so that the number of single GTO involved in a CGTO decreases with decreasing exponents as shown in Table 1, relaxing the contraction of the outer orbitals in going from atoms to molecules and solids in that order. To facilitate the forthcoming discussion, this prescription will be referred to as bond or free electron rule for molecules or metals respectively.

The constant factors multiplying each orbital present in a CGTO remain to be specified. The atomic calculations provide 1, 2, and 4 sets of expansion coefficients for the d, p, and s orbitals of copper respectively. In the absence of further exponent optimization in forming the CGTO one employs the atomic coefficients. The question is then the choice of the sets of coefficients to use. Given the exponents pertaining to the s symmetry, one has to choose among the expansion coefficients for the 1s, 2s, 3s, or 4s atomic states to form the CGTO describing the s symmetry functions. Basch et al. found the 1s atomic coefficients to describe all s orbitals far better than do the 3s coefficients. They mentioned a similar result reported by Huzinaga. Their finding has been verified for copper and nickel. This result could be expected, considering that the largest contribution to the total energy for a given symmetry is that belonging to the lowest principal quantum number, i.e., 1s for s, 2p for p, and 3d for d symmetries. This conclusion will be referred to as the lowest n rule. In the following all the CGTO have been
constructed using the 1s, 2p, 3d atomic coefficients for the s, p, and d orbitals.

If one utilizes the atomic coefficients as described above then elementary mathematics shows that grouping together two orbitals with expansion coefficients of different signs and exponents not far apart, is almost equivalent to eliminating them both as far as the charge density is concerned. The sign rule simply consists in avoiding such combinations.

In the Rayleigh-Ritz variational formalism the $m^{th}$ variational eigenvalue, $\lambda^{Nd}_m$ where Nd is the number of basis functions, tends to the true $m^{th}$ eigenvalue when Nd increases. Therefore, energy levels obtained with CGTO (reduced basis set) will generally not be lower than those generated using single GTO. A consequence of this is the upward shift of the energy levels to be expected when employing CGTO. This may appear as a drawback of the use of CGTO but should be of no effects on relative quantities such as exchange splittings and band widths resulting from solid state calculations.

The program package BNDPKG has been run to produce the non self-consistent energy levels of copper at high symmetry points of the Brillouin zone. The input for subroutine GTO determine the choice of contraction. The criterion for best contraction is the lowering of the energy levels. The above discussion of the limit behavior of variational eigenvalues as Nd increases makes it difficult to compare two contractions employing different numbers of CGTO. The 18 contractions in Table I, all of which involved 32 CGTO, has been used in these test calculations for copper. They are ranked in Table II from the best to the worst. One difficulty in choosing the overall
TABLE I. Contractions, eighteen different contractions (Nd = 32) used in the non self-consistent band calculations. The GTO utilized are those provided by Wachters. For a given symmetry the orbitals are numbered in the order of decreasing exponents.

<table>
<thead>
<tr>
<th>Contractions</th>
<th>S orbitals</th>
<th>P orbitals</th>
<th>D orbitals</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>(1,2,3,4,5,6) (7,8) (9) (10) (11) (12) (13)</td>
<td>(1,2,3,4,5,6) (7) (8) (9) (10)</td>
<td>(1,2,3,4) (5)</td>
</tr>
<tr>
<td>2</td>
<td>(1,2,3,4,5,6,7) (8) (9) (10) (11) (12) (13)</td>
<td>(1,2,3,4,5,6) (7) (8) (9) (10)</td>
<td>(1,2,3,4) (5)</td>
</tr>
<tr>
<td>3</td>
<td>&quot; &quot; &quot; &quot; &quot; &quot; &quot; &quot;</td>
<td>&quot; &quot; &quot; &quot; &quot; &quot; &quot; &quot;</td>
<td>(1,2,3) (4,5)</td>
</tr>
<tr>
<td>4</td>
<td>(1,2,3,4,5,6) (7) (8,9) (10) (11) (12) (13)</td>
<td>&quot; &quot; &quot; &quot; &quot; &quot; &quot; &quot;</td>
<td>&quot; &quot; &quot; &quot; &quot; &quot; &quot; &quot;</td>
</tr>
<tr>
<td>5</td>
<td>(1,2,3,4,5,6) (7) (8) (9,10) (11) (12) (13)</td>
<td>&quot; &quot; &quot; &quot; &quot; &quot; &quot; &quot;</td>
<td>&quot; &quot; &quot; &quot; &quot; &quot; &quot; &quot;</td>
</tr>
<tr>
<td>6</td>
<td>(1,2,3,4,5,6) (7,8) (9) (10) (11) (12) (13)</td>
<td>(1,2,3,4,5) (6,7) (8) (9) (10)</td>
<td>(1,2) (3,4,5)</td>
</tr>
<tr>
<td>7</td>
<td>&quot; &quot; &quot; &quot; &quot; &quot; &quot; &quot;</td>
<td>(1,2,3) (4,5) (6,7) (8,9) (10)</td>
<td>(1,2,3,4) (5)</td>
</tr>
<tr>
<td>8</td>
<td>&quot; &quot; &quot; &quot; &quot; &quot; &quot; &quot;</td>
<td>(1,2,3) (4,5) (6,7) (8) (9,10)</td>
<td>(1,2,3) (4,5)</td>
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<tr>
<td>9</td>
<td>&quot; &quot; &quot; &quot; &quot; &quot; &quot; &quot;</td>
<td>(1,2,3,4,5) (6,7) (8) (9,10)</td>
<td>&quot; &quot; &quot; &quot; &quot; &quot; &quot; &quot;</td>
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<tr>
<td>10</td>
<td>&quot; &quot; &quot; &quot; &quot; &quot; &quot; &quot;</td>
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<td>(1,2,3,4) (5)</td>
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<td>11</td>
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<td>12</td>
<td>&quot; &quot; &quot; &quot; &quot; &quot; &quot; &quot;</td>
<td>(1,2,3,4) (5,6) (7) (8,9) (10)</td>
<td>(1,2,3) (4,5)</td>
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<td>13</td>
<td>&quot; &quot; &quot; &quot; &quot; &quot; &quot; &quot;</td>
<td>(1,2,3,4,5) (6) (7) (8) (9,10)</td>
<td>(1,2) (3,4,5)</td>
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<td>14</td>
<td>&quot; &quot; &quot; &quot; &quot; &quot; &quot; &quot;</td>
<td>&quot; &quot; &quot; &quot; &quot; &quot; &quot; &quot;</td>
<td>(1,2,3) (4,5)</td>
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<tr>
<td>15</td>
<td>&quot; &quot; &quot; &quot; &quot; &quot; &quot; &quot;</td>
<td>&quot; &quot; &quot; &quot; &quot; &quot; &quot; &quot;</td>
<td>(1) (2,3,4,5)</td>
</tr>
<tr>
<td>16</td>
<td>&quot; &quot; &quot; &quot; &quot; &quot; &quot; &quot;</td>
<td>(1,2,3) (4,5) (6,7) (8,9) (10)</td>
<td>(1,2,3) (4,5)</td>
</tr>
<tr>
<td>17</td>
<td>&quot; &quot; &quot; &quot; &quot; &quot; &quot; &quot;</td>
<td>&quot; &quot; &quot; &quot; &quot; &quot; &quot; &quot;</td>
<td>(1,2) (3,4,5)</td>
</tr>
<tr>
<td>18</td>
<td>&quot; &quot; &quot; &quot; &quot; &quot; &quot; &quot;</td>
<td>&quot; &quot; &quot; &quot; &quot; &quot; &quot; &quot;</td>
<td>(1) (2,3,4,5)</td>
</tr>
</tbody>
</table>
TABLE II. Comparison of different contractions. The contractions are those in table I and are ranked from best to worst. The best is the one giving the lowest eigenvalues. The rankings change with symmetry points.

<table>
<thead>
<tr>
<th>States</th>
<th>Contraction Numbers</th>
<th>$\Delta_{max} = \max (\lambda^W_m - \lambda^B_m)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Core</td>
<td>1,4,5,2,3,8,9,6,11,10,14,12,13,15,7,16,17,18</td>
<td>+3.053 Ryd</td>
</tr>
<tr>
<td>S</td>
<td>1,7,10,8,9,11,12,14,16,6,13,15,17,18,2,3,4,5</td>
<td>+1.035</td>
</tr>
<tr>
<td>P</td>
<td>1,2,7,10,6,13,17,8,9,11,12,14,16,15,18,4,5,3</td>
<td>+0.011</td>
</tr>
<tr>
<td>$\Gamma$</td>
<td>1,2,3,4,6,8,9,5,11,7,10,13,17,16,14,15,18,12</td>
<td>+0.166</td>
</tr>
<tr>
<td>Valence Bands</td>
<td></td>
<td></td>
</tr>
<tr>
<td>L</td>
<td>1,2,3,4,5,6,8,9,11,10,7,12,14,13,15,16,17,18</td>
<td>+0.120</td>
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<tr>
<td>K</td>
<td>1,2,3,4,5,8,9,6,11,10,7,12,14,16,13,17,15,18</td>
<td>+0.111</td>
</tr>
<tr>
<td>X</td>
<td>1,2,3,4,5,6,8,11,9,10,12,13,14,15,7,16,17,18</td>
<td>+0.122</td>
</tr>
<tr>
<td>W</td>
<td>2,3,1,4,5,9,11,10,14,12,6,13,8,7,16,17,15,18</td>
<td></td>
</tr>
<tr>
<td>Higher Bands</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
best contraction is the change of the ranking from one state to another. One refers to the system specificities in order to make a choice. The electrical, thermal and optical properties of a metal being primarily determined by the valence and higher bands these levels will be considered the most important for copper. Let \( \lambda_m^b \) and \( \lambda_m^w \) designate the \( m^{th} \) eigenvalues obtained with the best and worst contractions, respectively. At the \( \Gamma \) point there exists 6 eigenvalues corresponding to the valence states (degeneracy included) of copper. The quantity

\[
\Delta_{\text{max}} = \max (\lambda_m^w - \lambda_m^b) ,
\]

(30)

where \( m \) takes 6 different values, has been used to compare the contractions. The values of \( \Delta_{\text{max}} \) in column 3 of Table II refer to the comparison of the best and worst contractions which are respectively the 1st and last ones as they appear in a row of Table II.

The detailed discussion of the contents of Table I and II is available in reference 71. With the knowledge that the twelfth 1s and the eight 2p orbitals have negative expansion coefficients the verification of the guidelines set above become apparent from these tables. Contractions 1-2 and to some extent 3-4, are the best for valence and higher bands while 15-18 are the worst for the same states. The best ones follow the guidelines best while the worst ones violate one or more of the rules. Interestingly, except for the deletion of the s tail and the inclusion of a tenth p orbital, contraction 14 corresponds to the best obtained by Wachters\textsuperscript{63} for
atomic copper. Contractions 1, 2, 3, and 4 are in this order, except at \( \Gamma \), for the valence states. This means \( A_{\text{max}} \) being relatively small at \( \Gamma \), that either one is expected to give good results.

The best contraction in Table II (contraction 1) has been chosen to perform self-consistent band structure calculations for FCC copper. At the exception of the contraction of the basis set every other parameter entering these computations has been kept as it was in the work of Bagayoko et al.\(^6\) where 75 GTO have constituted the basis set. Let \( \lambda_m^{32} \) and \( \lambda_m^{75} \) be the \( m \)th eigenvalues, beginning with the 1s state, resulting from the former and latter calculations. A detailed comparison of the valence bands for the high symmetry points, show:

\[
\lambda_m^{75} < \lambda_m^{32}, \quad E_F^{75} < E_F^{32}
\]

and

\[
\lambda_m^{75} - E_F^{75} = \lambda_m^{32} - E_F^{32} \pm 0.0025 \text{ Ry}, \quad (31)
\]

In the above expressions the Fermi energies \( E_F^{75} \) and \( E_F^{32} \) as well as \( \lambda_m^{75} \) and \( \lambda_m^{32} \) are negative quantities. This relation therefore shows that while the \( \lambda_m^{32} \) has been shifted upward as compared to the corresponding \( \lambda_m^{75} \), relative quantities like the occupied band widths have practically not been changed. This is the rigid upward shift (0.0142 Ry), due to the use of small basis set expected on variational grounds. The shift is illustrated by figure
Figure 2. Density of states $N(E)$ for paramagnetic FCC copper, in states/atom per Rydberg, obtained using bases of 75 and 32 GTO and CGTO respectively. The rigid upward shift of the bands for $N_d = 32$ is seen in the shift to the right of the Fermi level and the peaks in the density of states curve. $a = 6.80915$ a.u.
2 where the density of states resulting from both calculations are shown.

Another test of the guidelines for contraction is provided by the total energy calculation results. Not only a minimum is obtained in the total energy curve, but also it occurs around a lattice constant of 6.80915 a.u. which is almost identical to the experimental value for the equilibrium spacing at absolute zero. The above results on a 3d metal like copper leave no doubt about the adequacy of the above contraction procedure for the study of other 3d materials or lighter ones. The self-consistent calculations with 32 CGTO and 75 single GTO have been performed on an IBM 3033. The total CPU time required for the former was 6.8 times smaller than that (417 minutes) needed for the latter. This is the significant reduction of CPU time we were aiming for. Other miscellaneous benefits of this procedure are described in reference 71. In particular we have explicitly shown the inadequacy of some contractions for atoms and molecules in solid state calculations. BNDPKG has been used with a contraction option, following the above guidelines, to extensively study iron at 0°K. The results of those calculations are presented in the next chapter.
CHAPTER 4

ELECTRONIC STRUCTURES OF BCC AND FCC IRON

The new version of the band package, BNDPKG, has been used in this work. We employed the RSK local density potential. Choosing the contraction option of BNDPKG we constructed 8s,5p, and 4d CGTO according to the guidelines set forth in the preceding chapter. The atomic GTO entering the CGTO were those provided by Wachters. Only ferromagnetic inputs were considered and the ab-initio self-consistent band energies have been produced at 505 and 506 \( \vec{k} \) points of the respective irreducible wedges of the FCC and BCC structures. The input configurations, for both structures, were 3d\(^7\)4s\(^1\). These calculations have been carried out for several values of the atomic volume. The electronic structure of BCC iron at \( a = 5.4057 \) a.u. will be discussed in section A, followed by the studies of the variations of the bands with atomic volume for BCC and FCC lattices in sections B and C. The last section is devoted to the charge and spin form factors.

A. BCC Iron, \( a = 5.4057 \) a.u.

As previously stated most of the previous calculations for BCC iron at normal lattice constant (i.e., \( a = 5.4057 \) a.u., \( R_s = 2.6616 \) a.u.) are listed in the aforementioned references 1-6. A comparison of our results to those of Callaway and Wang is particularly meaningful as the differences between the two works reside in our use of 43 CGTO and the RSK potential instead of 75 GTO and the VBH
potential. The present calculations basically reproduced the results of Callaway and Wang. The present eigenenergies are rigidly shifted upwards as expected on variational grounds. However, in this case, contrary to the work on copper described in Chapter 3, the shift is primarily due to the use of a different method of evaluating $V_T(0)$. This Fourier coefficient of the Coulomb potential, as previously stated, does not affect the relative position of the bands. The algebraic values of the differences between the present and previous $V_T(0)$ and Fermi energies ($E_F$) are respectively 0.4376 and 0.4402 Ry. On the scales of the graphs in reference 2, the band structures these authors obtained are indistinguishable from ours if the Fermi levels are superposed. Tables III and IV contain major quantities describing these bands.

The magnetic moment, 2.15 $\mu_B$, is 0.01 $\mu_B$ less than the value they found. The up spin d band width at p is 2.5 eV, 0.2 eV less than their result. The exchange splitting at $P_4$, 1.31 eV, is 0.03 smaller than the previous value$^2$. We found charge and spin form factors almost identical to those obtained by Callaway and Wang. The analysis by Van Laar et al.$^{74}$ therefore shows than the spherical parts of both spin form factors are in accord with experiment. The above agreements between our results and previous theoretical as well as experimental ones justify the application of a contracted basis set to the study of iron at several atomic volumes. The slight reductions in the magnetic moment and the exchange splitting seem to indicate a somewhat stronger correlation effect in the RSK potential as compared to the WBH. Further discussion of the electronic structure of iron at normal lattice constant is presented in
conjunction with that of the variations of the bands with the lattice parameter.
Table III. Representative band widths (W) and exchange splittings ($\delta E_{\text{ex}}(P_{1})$) for BCC iron-in Rydbergs (Ry) - for various atomic radii ($R_g$), lattice constants (a) in a.u. Up or down spin is indicated by $+$ or $\pm$, respectively.

<table>
<thead>
<tr>
<th>$R_g$ (a.u.)</th>
<th>a (a.u.)</th>
<th>$W_{\text{sp}^{+}}$ ($H_{15}^{+} - \Gamma_{15}^{+}$) (Ry)</th>
<th>$W_{\text{d}^{+}}$ ($P_{3}^{+} - P_{4}^{+}$) (Ry)</th>
<th>$W_{\text{d}}$ ($P_{3}^{0} - P_{4}^{0}$) (Ry)</th>
<th>$\delta E_{\text{ex}}(\Gamma_{1})$ (Ry)</th>
<th>$\delta E_{\text{ex}}(P_{1})$ (Ry)</th>
<th>$\delta E_{\text{ex}}(P_{3})$ (Ry)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.4619</td>
<td>5.0</td>
<td>1.5533</td>
<td>0.2579</td>
<td>0.3262</td>
<td>0.4017</td>
<td>0.0176</td>
<td>0.0691</td>
</tr>
<tr>
<td>2.5603</td>
<td>5.2</td>
<td>1.4326</td>
<td>0.2165</td>
<td>0.2913</td>
<td>0.3798</td>
<td>0.0159</td>
<td>0.0794</td>
</tr>
<tr>
<td>2.6616</td>
<td>5.4057</td>
<td>1.3211</td>
<td>0.1822</td>
<td>0.2579</td>
<td>0.3540</td>
<td>0.0150</td>
<td>0.0855</td>
</tr>
<tr>
<td>2.7573</td>
<td>5.6</td>
<td>1.2269</td>
<td>0.1557</td>
<td>0.2310</td>
<td>0.3349</td>
<td>0.0147</td>
<td>0.0916</td>
</tr>
<tr>
<td>2.9542</td>
<td>6.0</td>
<td>1.0626</td>
<td>0.1114</td>
<td>0.1857</td>
<td>0.3094</td>
<td>0.0157</td>
<td>0.1079</td>
</tr>
<tr>
<td>3.4466</td>
<td>7.0</td>
<td>0.7742</td>
<td>0.0425</td>
<td>0.1141</td>
<td>0.2758</td>
<td>0.0212</td>
<td>0.1417</td>
</tr>
<tr>
<td>4.4313</td>
<td>9.0</td>
<td>0.3808</td>
<td>0.0062</td>
<td>0.0617</td>
<td>0.2792</td>
<td>0.0533</td>
<td>0.1881</td>
</tr>
</tbody>
</table>
Table IV. Representative band widths ($W$) and exchange splittings ($\delta E_{\text{ex}}$) for BCC-iron—in Rydbergs (Ry)—for various atomic radii ($R_s$) or lattice constants ($a$). $W_{\text{occ}}^d$ is the occupied $d$ band width. Up or down spin is indicated by $+$ or $-$, respectively.

$$
\begin{array}{cccccccc}
R_s & a & W_{\text{occ}}^d & W_{\text{d}}^+ & W_{\text{d}}^- & \delta E_{\text{ex}}(H_{12}^+ - H_{25}^-) & \delta E_{\text{ex}}(H_{12}^- - H_{25}^+) \\
(a.u.) & (a.u.) & (Ry) & (Ry) & (Ry) & (Ry) & (Ry) \\
\hline
2.4619 & 5.0 & 0.4602 & 0.5003 & 0.5287 & 0.0900 & 0.1183 \\
2.5603 & 5.2 & 0.4031 & 0.4159 & 0.4498 & 0.1054 & 0.1393 \\
2.6616 & 5.4057 & 0.3507 & 0.3435 & 0.3764 & 0.1169 & 0.1499 \\
2.7573 & 5.6 & 0.3091 & 0.2844 & 0.3151 & 0.1292 & 0.1599 \\
2.9542 & 6.0 & 0.2732 & 0.1838 & 0.2061 & 0.1612 & 0.1835 \\
3.4466 & 7.0 & 0.2421 & 0.0546 & 0.0419 & 0.2243 & 0.2116 \\
4.4313 & 9.0 & 0.2266 & 0.0002 & 0.0496 & 0.2729 & 0.2235 \\
\end{array}
$$
B. Volume Dependence of BCC Iron Band Structure

The up and down spin sub-bands of BCC iron at $a = 5.2$ a.u. in Figures 3 and 4 are shown to facilitate the forthcoming discussion. Figure 5 shows the total density of states. Fundamental parameters describing the bands, widths and exchange splittings, are provided in Tables III and IV.

Appendix B contains the valence state energy levels, at high symmetry points, for $a = 5.2, 5.4057,$ and $5.6$ a.u. The band widths decrease with increasing lattice constant and more up or down spin bands are respectively filled or emptied. These patterns can be described in terms of a competition between the kinetic and the exchange energies which get respectively smaller and larger in magnitude as the lattice constant increases.

One drastic change in the band structure of ferromagnetic BCC iron occurs at the $N$ point. For $a = 5.2$ a.u., Fig. 3, the upper $G_4$ and lower $D_3$ branches are connected to $N_1'$ which lies below $N_3$ where $G_2$ and the upper $D_3$ meet for the up spin sub-bands. In the down spin case, Fig. 4, $G_2$ and the upper $D_3$ meet at $N_3$ which lies above $N_4$ where the upper $G_4$ and $D_2$ are branching off. For the minority sub-bands this picture remains the same up to $a = 7.0$ a.u. where the upper $N_1, N_4,$ and $N_3$ are in that order of increasing energy but are almost degenerate ($E(N_4) - E(N_1) = 6.9$ mRy; $E(N_3) - E(N_4) = 5.6$ mRy). For the majority spin sub-bands $N_1'$ and $N_3$ become degenerate around $a = 5.4057$ (see Fig. 1 of Callaway and Wang\textsuperscript{2}, RS = 2.6616). This degeneracy no longer exists at $a = 5.6$ a.u. and above and the $G_2$ branch is connected to $D_3$ at $N_3$ which has moved below $N_1'$ where the upper $G_4$ and $D_3$ meet.
Figure 3. Energy bands in ferromagnetic BCC iron along some lines of high symmetry for the majority or up spin. Energies are in Rydberg (Ry). The lattice constant is $a = 5.2$ a.u.
Figure 4. Energy bands in ferromagnetic BCC iron along some lines of high symmetry for the minority or down spin. Energies are in Rydberg (Ry). The lattice constant is $a = 5.2$ a.u.
Figure 5. Total density of states $N(E)$, in states/atom per Rydberg, and the valence electron number for ferromagnetic BCC iron. The lattice constant is $a = 5.2$ a.u.
The passage of the $N_3$ representation below $N_1'$ in the majority spin sub-band is a direct consequence of the above mentioned competitions between kinetic and exchange energies. The $d$ states $(N_3)$ are far more sensitive to the exchange effect than are the $P$ ones $(N_1')$. When the lattice constant increases so does the exchange effect and $N_3$, for the up spin sub-bands, passes below $(N_1')$. There follows a change of connections to avoid the crossing of bands of the same symmetry, i.e., the upper and lower $D_3$.

A second major change in the structure of the $d$ bands is observed at a value of the lattice constant around 9 a.u. Figure 6 shows the up and down spin sub-bands for this lattice parameter at which the crystal field splitting is larger than the overlap effects; $t_{2g}$ and $e_g$ sub-bands are consequently split. It is apparent from figure 6 that the exchange splitting of the $d$ bands is then much larger than sub-band widths. In other words, the crystal field splitting is larger than the overlap effect and $t_{2g}$ and $e_g$ sub-bands are consequently split.

The values of the exchange splittings and band widths in Table III and IV, deserve comments. Callaway and Wang reported a rather large difference between the splittings at $P_4$ and $P_3$. This result has been reproduced here for $a = 5.4057$ as discussed in Section A of this chapter. One further observes, from Table III, that the increase of lattice constant is accompanied by a decrease of the ratio of the splitting at $P_3$ to that at $P_4$. For $a = 5.2$ a.u. this ratio is about 2; it tends to 1 as the lattice spacing increases because both splitting approach the same value which is that for the atoms. While the total $d$ band width at $P$, $W_d^{P}$, approaches that same atomic splitting, the widths for up and down spin sub-band go to zero. A known measure of the
Figure 6. Up (full) and down (dashed) spin energy bands of BCC iron at a lattice constant of 9.0 a.u. The following representations are in the order of increasing energy for both sub-bands:

\[ \Gamma_{25}^i, \Gamma_{12}^i; H_{25}^i, H_{12}^i; P_4, P_3. \]
hopping time for an electron occupying a given band is $\hbar/\omega$ where $\hbar$ is the Plank constant and $\omega$ is the band width. The smaller $\omega$, the more time the electron will spend on a given site. The relatively small d band widths as compared to the sp band widths is a result of the relative localization of the d electrons as compared to sp electrons.

A major characteristic of the BCC band structure of iron is the quasi-flatness of the $D_1, D_2, \Lambda_3$ and $\Sigma_4$ branches at lattice parameters equal or greater than 4.8 a.u. To this flat portion in the band corresponds a sharp peak in the density of state curve as shown in Fig. 5. These branches do not participate to the fermi surface. They therefore seem to possess a highly localized character as we shall discuss in connection with the study of the magnetic properties.

C. Electronic Structure of FCC Iron

The band structures of FCC iron at $a = 6.5516$ and 7.0 a.u. are shown in Figs. 7 through 10. Tables V and VI contain representative band widths and exchange splittings which describe variations of the bands with atomic volume. The valence band energies, at high symmetry points, can be found in Appendix B for the above lattice constants and $a = 6.8107$ a.u.

Drastic changes in the FCC band structure occur at the L point. In the majority spin sub-band $L_3$ and $L_2'$ are quasi degenerate$^{75}$ for $a = 6.8107$ a.u. ($R_s = 2.6616$); for smaller $R_s$ values, $L_2'$ lies below $L_3$ and the branchings are as in Fig. 7 ($a = 6.5516$ a.u.) while for larger ones $L_2'$ lies above $L_3$ and the branchings are as in Fig. 9 ($a = 7.0$ a.u.). A somewhat similar branch switching is described above for BCC iron.
Figure 7. Energy bands in ferromagnetic FCC iron along some lines of high symmetry for the majority or up spin. Energies are in Rydberg(Ry). The lattice constant is 6.5516 a.u.
Figure 8. Energy bands in ferromagnetic FCC iron along some lines of high symmetry for the minority spin. Energies are in Rydberg(Ry). The lattice constant is 6.5516 a.u.
Figure 9. Energy bands in ferromagnetic FCC iron along some lines of high symmetry for the majority or up spin. Energies are in Rydberg (Ry). The lattice constant is 7.0 a.u.
Figure 10. Energy bands in ferromagnetic FCC iron along some lines of high symmetry for the minority spin. Energies are in Rydberg (Ry). The lattice constant is 7.0 a.u.
Table V. Representative band widths (W) and exchange splittings ($\delta E_{ex}$) for FCC iron - in Rydbergs (Ry) - for various atomic radii ($R_a$) or lattice constants ($a$) in a.u. Up or down spin is indicated by + or - respectively.

<table>
<thead>
<tr>
<th>$R_a$ (a.u.)</th>
<th>$a$ (a.u.)</th>
<th>$W_{sp+}$ ($X_{4s+1}-X_{1s+1}$) (Ry)</th>
<th>$W_{d+}^X$ ($X_{2+2}-X_{3+1}$) (Ry)</th>
<th>$W_{d+d}$ ($X_{2+2}-X_{3+1}$) (Ry)</th>
<th>$\delta E_{ex}(X_{3+})$ (Ry)</th>
<th>$\delta E_{ex}(X_{2+})$ (Ry)</th>
<th>$\delta E_{ex}(f_{25+})$ (Ry)</th>
<th>$\delta E_{ex}(f_{12+})$ (Ry)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.1125</td>
<td>5.4057</td>
<td>1.3110</td>
<td>0.8316</td>
<td>0.8537</td>
<td>0.0094</td>
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<td>0.0224</td>
<td>0.0266</td>
</tr>
<tr>
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<td>0.7410</td>
<td>0.0141</td>
<td>0.0388</td>
<td>0.0286</td>
<td>0.0338</td>
</tr>
<tr>
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</tr>
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<td>2.5603</td>
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<td>0.8695</td>
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<td>0.0771</td>
<td>0.0918</td>
</tr>
<tr>
<td>2.6616</td>
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<td>0.0818</td>
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<tr>
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<td>0.2177</td>
<td>0.2315</td>
<td>0.2221</td>
<td>0.2278</td>
</tr>
</tbody>
</table>
Table VI. Representative band width ($W_d$) and exchange splittings ($\delta E_{ex}$) for FCC iron - in Rydbergs (Ry) - for various atomic radii ($R_s$) or lattice constants ($a$) in a.u.. $W_d^{\text{occ}}$ is the occupied d band width. Up or down spin is indicated by $\uparrow$ or $\downarrow$, respectively.

<table>
<thead>
<tr>
<th>$R_s$ (a.u.)</th>
<th>$a$ (a.u.)</th>
<th>$W_d^{\text{occ}}$ (Ry)</th>
<th>$W_d^{\uparrow}$ (X$<em>{5\uparrow}^-X</em>{1\uparrow}^+$) (Ry)</th>
<th>$W_d^{\downarrow}$ (X$<em>{5\downarrow}^-X</em>{1\downarrow}^+$) (Ry)</th>
<th>$\delta E_{ex}^{(L_3)}$ Lowest</th>
<th>$\delta E_{ex}^{(L_3)}$ Highest</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.1125</td>
<td>5.4057</td>
<td>0.7745</td>
<td>0.9629</td>
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</tr>
<tr>
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<td>0.0415</td>
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<tr>
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</tr>
<tr>
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<td>0.1218</td>
</tr>
<tr>
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<td>0.3376</td>
<td>0.3146</td>
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</tr>
<tr>
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<td>0.0636</td>
<td>0.1001</td>
<td>0.2237</td>
<td>0.2310</td>
</tr>
</tbody>
</table>
In both cases the representation reordering occurs around $R_5 = 2.6616$ a.u. and is limited to the majority sub-bands.

For lattice parameters less than 6.5516 a.u. the exchange splittings of the two uppermost d bands ($A_3$ branches included), almost constant in the zone, double for 0.5 a.u. increase while for values above 7.0 a.u. the splittings change by less than 10% for such increase. At $a = 6.5515$ a.u. the ratio of the splitting to the width for these bands are around 1/3 while their values are slightly less or greater than one for the lower and upper (as at W) ones at $a = 7.0$ a.u. If one limits consideration to the W-L-Γ branches of these bands one still finds the ratio less than one for both bands at $a = 6.5516$ a.u. while it is greater than one for both at $a = 7.0$ a.u. The above points are particularly meaningful for the up spin sub-bands. The two uppermost d bands for the minority spin are either empty or clearly participate to the Fermi surface. However, for lattice spacings equal to or greater than 7.0 a.u. these bands are fully occupied for the majority spin. The above discussion, the first of its kind on the details of the band structures of iron will be of importance in the understanding of the magnetic properties of this metal. Some by-products of these band structure calculations, using BNKPKG, are the charge and spin form factors. We shall discuss these in the next section.

D. BCC and FCC Iron Form Factors

The x-rays and neutron scattering form factors are gauge of the quality of the wave functions resulting from calculations as the present. This is so because these quantities, also respectively
referred to as charge \( f_c \) and spin \( f_s \) form factors, are directly related to the Fourier transform of the charge density:

\[
f_c(k, \ell, m) = \rho(k, \ell, m) \cdot \Omega
\]

and

\[
f_s(k, \ell, m) = \frac{\rho_+(k, \ell, m) - \rho_-(k, \ell, m)}{\rho_+(0,0,0) - \rho_-(0,0,0)}
\]

In these expressions \( \Omega \) is the cell volume and \( \rho(k, \ell, m) \) stands for the Fourier transforms of the charge density with \( k, \ell, m \) designating the \( x, y, \) and \( z \) components of the reciprocal lattice vectors in units of \( 2\pi/a \). Charge and spin form factors of BCC iron are in Tables VII through IX for \( a = 5.0, 5.4057, \) and \( 6.0 \) while those of FCC iron are in Tables X through XII for \( a = 6.5516, 6.8107, 7.0 \) a.u. It is to be recalled that Van Laar and coworkers\(^7\) have established that the spin form factors for BCC iron for \( a = 5.4057 \), which are the same as those provided by Callaway and Wang\(^2\), agree with experiment. The content of Table X-XII constitutes the first, at the author's knowledge, published form factors for FCC iron.

These data are provided for three different lattice parameters in order to allow much better comparison with experiment. Indeed, several tests have revealed that over a range of \( 1 \) a.u., the form factors can be fitted to a polynomial in \( a \) (lattice constant) of degree two for a given \( \ell_S \) vector:

\[
f_c(k, \ell, m) = a_0^{c,k \ell m} + a_1^{c,k \ell m} \cdot a + a_2^{c,k \ell m} \cdot a^2
\]
Table VII. The charge ($f_c$) and spin ($f_s$) form factors for BCC iron.

The coordinates $k$, $\ell$, $m$ of the reciprocal lattice vectors are in units of $\frac{2\pi}{a}$. $a = 5.0$ a.u.

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Table VIII. The charge ($f_c$) and spin ($f_s$) form factors for BCC iron.

The coordinates $k$, $\ell$, $m$ of the reciprocal lattice vectors are in units of $\frac{2\pi}{a}$. $a = 5.4057$ a.u.

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Table IX. The charge \((f_c)\) and spin \((f_s)\) form factors for BCC iron.

The coordinates \(k, \ell, m\) of the reciprocal lattice vectors are in units of \(\frac{2\pi}{a}\). \(a = 6.00\) a.u.

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Table X. The charge \((f_c)\) and spin \((f_s)\) form factors for FCC iron.

The coordinates \(k, \ell, m\) of the reciprocal lattice vectors are in units of \(\frac{2\pi}{a}\). \(a = 6.5516\) a.u.

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Table XI. The charge \( f_c \) and spin \( f_s \) form factors for FCC iron.

The coordinates \( k, \ell, m \) of the reciprocal lattice vectors are in units of \( \frac{2\pi}{a} \). \( a = 6.8107 \) a.u.

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Table XII. The charge ($f_c$) and spin ($f_s$) form factors for FCC iron.

The coordinates $k$, $\ell$, $m$ of the reciprocal lattice vectors are in units of $\frac{2\pi}{a}$. $a = 7.0$ a.u.

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and

\[ f_s(k, \lambda, \mu) = a_{0,k\lambda \mu}^s + a_{1,k\lambda \mu}^s \lambda + a_{2,k\lambda \mu}^s \lambda^2 \]  \hspace{1cm} (33)

The relevant coefficients, \( a_i^c \) or \( a_i^s \) are provided in Appendix B for the BCC iron form factors in Tables VII through IX. It is easily verified that the contents of these tables are exactly reproduced by these fits. Intermediate values, i.e., the form factors at \( a = 5.2 \), are obtained well beyond the second decimal place. Clearly, this signifies that experimental form factors can be judiciously compared to the theoretical ones for a lattice parameter equal to that existing in the conditions of measurements (i.e., non-zero temperature). The above locally quadratic dependence of the form factors of BCC or FCC iron is not unique to this metal. It applies equally well to lithium and copper.
The present calculations, with ferromagnetic inputs, resulted in magnetic moments, for BCC and FCC iron which are plotted in Fig. 11 versus $R_s$. Table XIII displays the moments, the density of state at the Fermi level as well as the characteristic exchange splittings. The latters are the energy differences between the absolute maxima in the majority and minority spin density of state curves. Density of states curves for FCC iron at $a = 6.5516$, $6.8107$, and $7.0$ a.u. are respectively shown in Figures 12, 13, and 14.

BNDPKG yields from a ferromagnetic input a paramagnetic ordering provided the latter is the most stable one. In light of this, Fig. 11 indicates that BCC and FCC iron are not paramagnetic for the $R_s$ values in the range considered. These calculations predict ferromagnetism for BCC and FCC iron but they do not exclude antiferromagnetism\textsuperscript{32} (in FCC iron) which is not addressed here.

The first section of this chapter is devoted to the discussion of the results in Table XIII and Fig. 11. The following sections, B and C address the relevance of our findings to properties of some iron based alloys after a comparison with experiment.

A. Ferromagnetism in BCC and FCC Iron

Figure 11 indicates a rather smooth variation of the magnetic moment per atom in BCC iron for $R_s$ values greater or equal to
Figure 11. The magnetic moment, in Bohr magneton, versus Wigner-Seitz radius ($R_s$), in atomic units (a.u.), for BCC (dashed curve) and FCC (full curve) iron.
Table XIII. Density of states (states/atom-Rydberg) for majority (+) and minority (−) spin electron at the Fermi energy

\( (\text{Rydberg-atom}^{-1}) \), magnetic moment per atom (in Bohr magneton) \( m \), and the characteristic exchange splitting delta \( \Delta_c \) in Rydberg (Ry) for BCC and FCC iron.

<table>
<thead>
<tr>
<th>( R_s )</th>
<th>( N_+ (E_F) )</th>
<th>( N_- (E_F) )</th>
<th>( m )</th>
<th>( \Delta_c )</th>
<th>( R_s )</th>
<th>( N_+ (E_F) )</th>
<th>( N_- (E_F) )</th>
<th>( m )</th>
<th>( \Delta_c )</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.462</td>
<td>8.321</td>
<td>6.736</td>
<td>1.735</td>
<td>0.142</td>
<td>2.112</td>
<td>5.219</td>
<td>5.206</td>
<td>0.126</td>
<td>0.017</td>
</tr>
<tr>
<td>2.560</td>
<td>9.263</td>
<td>3.892</td>
<td>1.987</td>
<td>0.162</td>
<td>2.188</td>
<td>5.985</td>
<td>5.832</td>
<td>0.186</td>
<td>0.042</td>
</tr>
<tr>
<td>2.661</td>
<td>11.036</td>
<td>3.341</td>
<td>2.153</td>
<td>0.172</td>
<td>2.345</td>
<td>7.839</td>
<td>9.140</td>
<td>0.397</td>
<td>0.057</td>
</tr>
<tr>
<td>2.757</td>
<td>13.906</td>
<td>4.802</td>
<td>2.317</td>
<td>0.177</td>
<td>2.560</td>
<td>12.068</td>
<td>10.097</td>
<td>0.966</td>
<td>0.090</td>
</tr>
<tr>
<td>2.954</td>
<td>19.649</td>
<td>2.717</td>
<td>0.197</td>
<td></td>
<td>2.661</td>
<td>23.826</td>
<td>10.330</td>
<td>1.517</td>
<td>0.120</td>
</tr>
<tr>
<td>3.447</td>
<td>2.923</td>
<td>60.269</td>
<td>3.269</td>
<td>0.232</td>
<td>2.736</td>
<td>2.470</td>
<td>13.346</td>
<td>2.549</td>
<td>0.187</td>
</tr>
<tr>
<td>4.431</td>
<td>1.106</td>
<td>484.124</td>
<td>3.943</td>
<td>0.277</td>
<td>3.517</td>
<td>2.739</td>
<td>36.140</td>
<td>3.359</td>
<td>0.215</td>
</tr>
</tbody>
</table>
Figure 12. Total density of states $N(E)$, in states/atom per Rydberg, and the valence electron number for ferromagnetic FCC iron. The lattice constant is $a = 6.5516$ a.u.
Figure 13. Total density of states $N(E)$, in states/atom per Rydberg, and the valence electron number for ferromagnetic FCC iron. The lattice constant is $a = 6.8107$ a.u.
Figure 14. Total density of states $N(E)$, in states/atom per Rydberg, and the valence electron number for ferromagnetic FCC iron. The lattice constant is $a = 7.0$ a.u.
2.462 a.u. This behavior of the moment is explained, in general terms, by the gradual and continuously filling of the majority spin bands as compared to the minority ones. Due in part to the increase of the exchange effect, the majority spin bands are lowered with respect to the Fermi level while the minority energy levels are pushed upwards. BCC iron becomes a strong ferromagnet between the lattice constants of 5.6 and 6.0 a.u. This corresponds to the sinking below $E_F$ of the $G_2$ branch in the up spin band. The smooth increase of the moment is basically the result of the progressive (see Fig. 4) transfer of electrons from the minority spin bands. A drastic change is not observed simply because no flat band crosses the Fermi level. We recall that the relatively flat bands in the structure, at ordinary lattice parameters, are the two uppermost d bands ($D_1$, $D_2$, $A_3$, and $E_4$ branches) which, as previously stated are respectively full or empty for the majority or minority sub-bands. This behavior of the bands, which fully explain the moment versus $R_s$ curve of BCC iron is not unique to this metal.

Walmsley and coworker\textsuperscript{76} recently have grown a BCC cobalt film, for the first time, on a chromium substrate. The moment was believed to be around that of the ordinarily stable HCP phase of this metal. Bagayoko, et al.\textsuperscript{77} performed ab-initio band structure calculations on this novel phase of cobalt at lattice constants of 5.0, 5.2346 (experimental value), 5.3099 and 5.4456 a.u. The magnetic moments these authors reported, as shown in Table XIV, behave like those of BCC iron when the atomic volume changes. The flat bands which are believed to play a stabilizing role as to the variation of the moment are equally below and above the Fermi level, for up and down spin respectively, for the lattice constants considered. Like the case of BCC iron, no drastic
TABLE XIV. The magnetic moment ($m$, in Bohr magneton) for BCC cobalt at various atomic radii ($R_s$) or lattice constants ($a$) in atomic units (a.u.).

<table>
<thead>
<tr>
<th>$R_s$ (a.u.)</th>
<th>$a$ (a.u.)</th>
<th>$m$ ($\mu_B$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.4619</td>
<td>5.0</td>
<td>1.545</td>
</tr>
<tr>
<td>2.5774</td>
<td>5.2346</td>
<td>1.646</td>
</tr>
<tr>
<td>2.6144</td>
<td>5.3099</td>
<td>1.678</td>
</tr>
<tr>
<td>2.6813</td>
<td>5.4456</td>
<td>1.736</td>
</tr>
</tbody>
</table>
change with lattice parameter is expected for values of the latters above 5.0 a.u.

This behavior of the magnetic moment of BCC iron is quite similar to that of FCC iron at lattice parameters above 7.0 a.u. Figure 11 shows the two curves become indistinguishable between the $R_s$ values of 3.25 and 3.75 a.u. However, the magnetic moment of FCC iron for $R_s$ values below 2.73 (a less than 7.0 a.u.) behave quite differently than does the BCC moment. There is a rather steep rise of the moment around $R_s = 2.71$ a.u. This has been first observed theoretically by Madsen and Andersen; these authors found a different $R_s$ value for the transition ($R_s \approx 2.61$ a.u.). This transition has been very recently explained in terms of the band structures by Bagayoko and Callaway. The following explanation parallels the one given by these authors.

A relatively flat portion of the uppermost up spin d band, see Fig. 7, crosses the Fermi level for $a = 6.5516$ a.u. Specifically we are referring to the $z_2$, uppermost $Q_1$ and $A_3$ branches. These branches, as shown in Fig. 8, are above the Fermi level in the minority spin bands for the same lattice constant. The combination of the increase of the exchange effect and the decrease of kinetic energy lower these branches, in the majority sub-bands, while it pushes them upwards in the down spin bands, relative to the Fermi level as the lattice parameter increases. For the majority spin these branches are below $E_F$ at $a = 7.0$ a.u. The abrupt increase in the magnetic moment of FCC iron when the lattice constant change from 6.5516 to 7.0 is due to this transition, i.e., the passage of the uppermost up spin d bands below the Fermi energy and the subsequent disappearance of portions of the Fermi surface. This transition is continuous in the sense that these bands progressively
sink below the Fermi level.

There is a second aspect of this transition equally as important as the filling of these up spin bands, i.e., the increased flatness of the bands which is the manifestation of a relative localization. We have observed, see Figs. 7 through 10, that the ratio of the exchange splitting to the width of the uppermost d bands in FCC iron is less than unity for lattice constants less than or equal to 6.516 a.u. This ratio is a quantitative measure of the degree of flatness of these bands. For $R_s$ values above 2.73 a.u., the ratio is greater than one, indicating relatively flat bands or an increase in atomic character of the electrons occupying them. As explained in the discussion of the magnetic properties of BCC iron, once these flattened d bands lie below $E_F$, in the majority spin, no drastic variation of the moment with lattice parameter is expected, because the corresponding ones in the minority spin bands are above the Fermi energy. Bagayoko and Callaway estimated the transition atomic radius to be $R_s = 2.71$ a.u. At the transition atomic volume $Z_2$ branch is expected to lie at the Fermi level in the up spin sub-band.

The data in Table XIII show the onset of the transition to strong ferromagnetism for BCC and FCC iron. In both cases it is indicated by a relatively large density of down spin states as compared to that for the up spin ones at the Fermi level. Figures 12, 13 and 14 illustrate the same transition for FCC iron. It should be noted that while these figures are indicative of the establishment of strong ferromagnetism, one needs the detail band structure to ascertain the otherwise conjectural observation.

If the moment of BCC cobalt behaves like that of BCC iron for
varying atomic volume, the situation in nickel seems to resemble that of FCC iron. Indeed, Wang and Callaway\textsuperscript{54} presented the band structure of this 3d metal for a lattice constant of 6.644 a.u. Weling and Callaway\textsuperscript{78} produced semi-empirical bands of FCC nickel which fitted the experimentally observed\textsuperscript{79} structure. Bagayoko\textsuperscript{73}, in the course of testing the new version of BTKPKG obtained results qualitatively similar to those of Wang and Callaway\textsuperscript{54}. The magnetic moment obtained by the various calculations is around 0.55 $\mu_B$. The important feature of the structures of FCC nickel of particular interest here is the itinerant character they possess as compared to BCC iron. The ratio of the exchange splitting to the total individual widths for the uppermost d bands of nickel ($a = 6.644$ a.u.) is less than one; a result similar to that found for FCC iron at $a = 6.5516$ a.u. However, if one considers only the $\Gamma$-$L$-$W$ branches of these bands, in calculating the widths, the above ratio remains less than 1 for the down spin cases and becomes greater than one for the uppermost up spin ($\Gamma_{12}^{-}$-$L_{3}^{-}$-$W_{1}^{+}$) in the case of nickel.

B. Comparison with Experiment

Our prediction of ferromagnetism for FCC iron is in agreement with the most recent experimental conclusions\textsuperscript{17,25} as we shall discuss. At first a comparison with the theoretical works seems appropriate.

Andersen and coworkers\textsuperscript{31} reported two different results on the magnetic ordering in FCC iron. Madsen and Andersen\textsuperscript{29} found FCC iron to be ferromagnetic for $R_s$ values above 2.47 while Poulsen \textit{et al.}\textsuperscript{30} found a non-zero moment only for $R_s$ larger than 2.6 a.u. Poulsen \textit{et al.}, unlike Madsen and Andersen, included the sp-d hybridization in all their
calculations. The zero moment result of Poulsen et al. could be attributed to an overestimate of the correction to the unhybridized results. The drastic changes in the d band branchings as described here are indeed difficult to account for by the positioning and scaling of the projected density of states as was done by Madsen and Andersen or Poulsen et al. when the sp-d hybridization is included. The rather good results these authors obtained for normal volume (i.e., a magnetic moment of 2.17 \( \mu_B \)) do not contradict the above contention as a full band structure calculation was used in that case instead of scaling procedures.

Bagayoko and Callaway\textsuperscript{75} recently discussed the results of Kubler\textsuperscript{32}. There is a qualitative agreement between this author's results and ours on the ferromagnetism of FCC iron below \( R_s = 2.60 \). There exist quantitative differences. In particular we find the moment not to vanish at \( R_s = 2.50 \) a.u. and we place the abrupt increase of the moment of FCC iron around \( R_s = 2.71 \) instead of about 2.645 a.u. The total energy curves obtained by Kubler indicate the stable phase of this metal to be an anti-ferromagnetic FCC, contrary to experiment, for \( R_s \) values between 2.5 and 2.7 a.u. The spherical averaging of the charge density inherent to the augmented spherical wave method is suspected\textsuperscript{32} to cause this problem.

Roy and Pettifor\textsuperscript{34} found the Tauer and Weiss \( \gamma_1 \) and \( \gamma_2 \) states to be both ferromagnetic. Their unhybridized ASA calculations are therefore in qualitative agreement with our results. However we should emphasize the continuity in the steep rise of the moment between \( R_s = 2.56 \) and \( R_s = 2.736 \) a.u. which is apparent from Fig. 1 as opposed to the discontinuity implied by the original \( \gamma_1 \) (antiferromagnetic) and \( \gamma_2 \)
(ferromagnetic) hypothesis. Even though it is difficult to draw a conclusion from Kubler's results, several experimental ones found antiferromagnetic FCC iron at some $R_s$ value less than 2.76.

As discussed in the first chapter, the magnetic ordering in FCC iron is suspected to depend on both film orientation and atomic separation. The difficulty connected with the experimental determination of the lattice constant compounds the problem. Still the results of Wright seem to be in good agreement with ours. This author found a ferromagnetic $\gamma$ Fe film to possess a moment of 1.1 $\mu_B$, for a lattice spacing estimated to be 6.8 a.u. At a lattice constant of 6.8107 a.u. the present result shows a moment of 1.517 $\mu_B$. Considering that 6.8 a.u. was an upper limit for the experimental value and the rapid variation of the moment around this lattice parameter, this appears as a good agreement between experiment and theory. Gonser et al. estimated a transition from anti-ferromagnetism to ferromagnetism to occur between $R_s = 2.67$ and $R_s = 2.78$ a.u. These authors, as mentioned in the introduction, found FCC iron precipitate in Cu$_{59}$Au$_{30}$ to be ferromagnetic. We found the atomic radius for the transition to strong ferromagnetism to be about 2.71 a.u. for FCC iron. Their estimate of the smallest $R_s$ value (2.67) compatible with ferromagnetism in FCC iron seems to be in disagreement with Wright's result where ferromagnetism is found at an $R_s$ value below 2.66 a.u. The difficulties in the evaluation of the lattice parameter, due in part to possible pseudomorphic phase for the film, could account for the difference and vindicate either finding.

C. Relevance to Iron Based Alloys
The present study of ferromagnetic γ iron is quite relevant to the properties of FCC iron based alloys in general and the invar alloys in particular. That is so in part because at most two shells of neighboring iron atoms are believed to be needed for the central atom to exhibit bulk properties\(^\text{32}\).

The most recent explanations of the invar anomalies do not assume γ iron to be antiferromagnetic\(^\text{21,80,81,82}\). While the explanation of Kaspar and Salahub\(^\text{21}\) assume ferromagnetic order, Gavoille\(^\text{82}\) reaches the conclusion that antiferromagnetically coupled iron atoms cannot be responsible for invar phenomena. The band structure of FCC iron in Fig. 7 through 10 could be used to support arguments of the type presented by Kaspar and Salahub. These authors obtained the ferromagnetic energy levels of Fe\(_{13}\), Fe\(_{12}\)Ni and Ni\(_{13}\) clusters; the respective non-bonding and anti-bonding characters of the minority and majority spin sub-levels just above the Fermi level (\(E_F\)) are used to discuss invar effects in Fe\(_{64}\) Ni\(_{36}\) (for Ni concentrations around 35\%) through filling and emptying of levels. Two factors entering the analysis are the smaller atomic volume and excess electrons (2) nickel possesses as compared to iron. Hattox and coworkers\(^\text{83}\) studies some properties of BCC vanadium as a function of the lattice constant. They described the possible usefulness as well as the limitations of the properties of pure metals in understanding alloys. The relevance of the present results to a complete theory of invar phenomena is illustrated by the work of Shiga\(^\text{84}\) who studied the magneto-volume invar effects for Fe-Ni alloys among others. This author fits rather well the lattice constant (\(a(X)\)) versus nickel concentration (\(X\)) curves of Fe-Ni alloys with a modified Vegard's Law:
\[ a(X) = a_1 (1 - X) + a_2 X + c \mu(X) \]

where \(a_1\), \(a_2\) and \(c\) are adjustable parameters and \(\mu(X)\) an average atomic moment. At absolute zero the curve shows the maximum lattice constant for the alloy to be about 6.77 a.u. at approximately 38% nickel; this spacing is in the region of steep rise of the moment of FCC iron. The deviations from the Vegard's Law are attributed to a magnetic contribution to the expansion as recently discussed by Morruzi et al.\(^6\) for pure metals.
CHAPTER 6
DISCUSSION AND SUMMARY

It is apparent from the survey of previous works as well as the preceding description of magnetism in BCC and FCC iron that the present results and their analysis could be of importance for future investigations. We shall elaborate on such investigations as they appear through further discussion in section A. We present a summary of our findings in section B.

A. Discussion for Future Work

While experiments agree on the absence of paramagnetism in FCC iron, as found here, they disagree somewhat on the magnetic ordering in this metal. Antiferromagnetism\textsuperscript{11,24} and ferromagnetism\textsuperscript{17,22,23,25} are found in both gamma iron precipitates and films. Film orientation\textsuperscript{24} or atomic separation\textsuperscript{25} are suggested to be factors determining the magnetic order in FCC iron. However, we mentioned the observation of ferromagnetism in iron film\textsuperscript{22} at a lattice constant smaller than the minimum required, according to Gonser et al.,\textsuperscript{25} for the establishment of this magnetic ordering. The present results could allow meaningful comparison with experimental ones provided progress is made in the determination of the atomic separation in films or precipitates.

A first possible continuation of this work would be to extend the band package, BNDPKG, in order to produce the band structure of materials with two atoms per cell. The treatment of antiferromagnetism requires such a modification. These changes could be made in a manner
to allow for the calculation of the total energy. Although it might still be difficult to accommodate such factors as pseudomorphism in films or defects, this will permit the determination, from the total energy curve, of the most stable ordering at a given atomic volume for the pure metal. This is needed because any inference of the stability of the antiferromagnetic ordering from Kubler's results requires iron to be in the FCC structure, contrary to reality, in ordinary conditions of temperature and pressure.

These total energy calculations could be supplemented by the concomitant evaluation of the pressure. Indeed the infinite terms which appear in the expression of the pressure as given by Janak are easily avoided by expressing the Coulomb contributions to the potential energy in terms of \( U \) and \( D \) as defined in Chapter 2. This of importance as previous evaluation of the pressure necessitated approximations, like the Muffin-Tin one, in order to avoid divergences. All the required entities are obtained in the process of band structure calculations using the new version of BNDPKG as shown in appendix c.

The above total energy and pressure calculations might require an large amount of CPU time for iron due to a slow convergence of the sums in \( U \) and \( D \) as defined in Chapter 2. This is so because of the very large gaussian exponents used to describe the core and also the nuclear repulsion term in the potential. In the work on copper the sums had to be carried out to a value of the square of \( K_S \) over 12,000 to obtain convergence. Such a summation appears impractical at over 20 lattice parameters as would be the case here for iron. Based on the rather slow variations of the Fourier coefficients at large \( K_S \) values one could replace the sums by integrals. This non-trivial honing of the total
energy calculation procedure is not only of potential use in the above suggested work on iron but also will enable one to study, from band calculations, the central pair potentials as described by Matthai et al.\textsuperscript{86} and March\textsuperscript{87}. Besides their obvious usefulness in metallurgy, these pair potentials can be applied to the study of defects.\textsuperscript{87}

An important result obtained here has been the observation of the atomic behavior of some valence states in BCC iron. In FCC iron we have similar results for lattice constants above 7.0 a.u. These characteristics show up in the values and variations of the band widths and exchange splittings. Experimental\textsuperscript{88} and theoretical\textsuperscript{89} works intimated these results. In particular, Stearns\textsuperscript{88} obtained evidence for quasi-localized states in BCC iron as well as other 3d metals which are hybridized with itinerant or continuum ones. The shake up structures observed in nickel\textsuperscript{79} could be seen as further confirmation of Stearn's\textsuperscript{88} observations. The increased directionality\textsuperscript{86} from FCC to HCP and BCC, in that order, implied a somewhat atomic character in BCC iron. A more direct observation of this fact was the failure of the cluster approach calculation to yield an acceptable value of the critical temperature ($T_c$) of iron for any size of the cluster. On the contrary, Ziegler\textsuperscript{89} reproduced the experimental value of this quantity for nickel.

Despite the above wealth of information on the localization of valence electrons in BCC iron, a detailed conceptual understanding of it is not yet available. It is not clear what interpretation one can give to parabola like portions of the bands they occupy. Various forms of hybridization (sp-d, d-d) can be invoked but lack a firm footing.

The data obtained here can be used to compute the probability that an electron occupying a band no at a given site at time $t$ be found at
time $t'$ at another site. The basic formalism to do this has been provided by Callaway and Hughes in their study of localized defects in semi-conductors using Wannier functions. Such transition time or probability will allow a quantitative description of the degree of localization at any lattice constant.

The above suggested experimental as well as theoretical works can benefit from our findings. In particular most computations we mentioned can use the present data as input. Other studies as those of the Compton profile, the Fermi surface, or the optical conductivity can, in a straightforward manner, utilize the results we wish to summarize in the following section.

B. Summary

We have reviewed previous theoretical and experimental works on BCC and FCC iron. A new formalism for the calculation of the total energy and pressure of a metal has been described. We extended Wang and Callaway's program package in order to implement this formalism. We described the general and new features of this package, BNDPKG, which utilizes Gaussian basis in a LCAO scheme. Local density potentials (i.e., VBH, RSK) are allowed for in BNDPKG. The large size of the Hamiltonian matrix resulting from the use of GTO or CGTO led to a careful study of contraction of basis sets. The most important successful test of the guidelines set forth for contraction has been the obtention of a minimum, at about the experimental lattice constant, in the total energy curve of FCC copper, a 3d metal. The large reduction of CPU time resulting from the use of CGTO opened the way for the present detailed study of the electronic structure of BCC and FCC iron.
Keeping in sight possible extensions of this work, as suggested above (i.e., total energy and pressure calculation), we employed the new version of BNDPKG. The band widths and exchange splittings discussed quantitatively described the variations of the electronic states in BCC and FCC iron as the lattice constant changes. The decrease or increase of the band width or the exchange splitting as the lattice parameter increases is explained by the competition between the kinetic and exchange energies. Several features of the electronic structures of iron have been reported here for the first time. In particular the reordering of representations in the band structure of BCC and FCC iron was described. This reordering, which occurs for both structures around \( R_s = 2.6616 \) a.u., is accompanied by changes of branching of the band to avoid forbidden crossings. This branch switching is suspected of being a contributing factor to the difference between the results of Madsen and Andersen and Poulsen et al.

While ferromagnetism in BCC iron was found to possess an atomic origin due to characteristically flat portions of the d bands, the results for FCC iron are mixed. We explained, using ab-initio self-consistent band structures, the abrupt jump in the magnetic moment of FCC iron when \( R_s \) varies from 6.5516 to 7.0 a.u. This jump is found to be the result of the establishment of strong ferromagnetism in FCC iron. We emphasized the increased flatness of the top d bands in FCC iron for \( R_s \) values above the transition point (\( R_s = 2.71 \) a.u.). For very large lattice constants we found the moment in both structures to behave similarly. We found in BCC iron, at lattice constants above 9.0 a.u., the crystal field splitting to be larger than the overlap effects. The forms factors we obtained as well as their locally
quadratic dependence on the lattice constant could be of use in the analysis of experimental works. BCC cobalt has been predicted to behave, as far as the moment variation with $R_s$ is concerned, like iron. The reasons for this were given in terms of the band structure. We indicated the usefulness of our results in a complete understanding of iron alloys in general and the invar alloys in particular. We mentioned few of the many possible future works, experimental or theoretical, for which the results of this work, presented or available, could play a role of reference material.
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87. N. M. March to be published.
91. Supplementary data available upon request from D. Bagayoko or J. Callaway.
APPENDIX A.1: New Version of PROGRAM FCOF

DSN=PhBAGA_DIOOLA_FCOF

//PEF1B60 JOB (1103,72121,20,2), 'Ph.DIOOLA', MSGLEVEL=1,
// NOTIFY=PhBAGA
//*AFTER PEF1B060
//*JOBPARM SHIFT=1
//*ROUTE PRINT PHYSICS
//*A EXEC FORTHCLG,PARM.FORT='NOSOURCE,LANGIVL(66),OPT(2)',
//* PARM.LNXD=NOIBM,REGION=1200K,TIME=999
//*FORT,SYSIN DD *

PROGRAM FCOF
THE FIRST PART OF
A GENERAL PROGRAM TO CALCULATE SELF-CONSISTANT ENERGY BANDS
USING THE MODIFIED TIGHT BINDING OR LCGC METHOD
BY
C.S. WANG AND J. CALLAWAY
EXTENSION FOR TOTAL ENERGY CALCULATIONS
BY
J. CALLAWAY, X. ZOU, AND D. BAGAYOKO
DEPARTMENT OF PHYSICS
LOUISIANA STATE UNIVERSITY
BATON ROUGE LOUISIANA 70803

COMMON BLOCKS OCCURING IN FCOF

Routines Used in FCOF
FCG TOTAL ENERGY CALCULATION

ATDENS
CPHYG
COULON
FILON
GBZPT
GLFDFK
GMIS
GPEREK
GRADPT
OPENAD
POEXCH
SPHNT
TELECT
VXCRS1

COMMON, SIS, ROUTINES IN WHICH THEY ARE USED

CHARGE ATDENS, FCGF, OPENAD, POEXCH
CONS1 ATDENS, COULON, FCGF, OPENAD, POEXCH
END FCOF, OPENAD
FOURIER COEFFICIENTS OF THE COULOMB AND EXCHANGE POTENTIAL.
GAUSSIAN TYPE WAVE FUNCTIONS ARE USED IN THIS PROGRAM.
THE FOURIER COEFFICIENTS OF THE COULOMB POTENTIAL ARE EVALUATED
ANALYTICALLY.

THE EXCHANGE POTENTIAL IS EVALUATED IN THE FOLLOWING WAY.
EACH ATOM IS SURROUNDED BY TWO SPHERES OF RADIUS ROGAUS AND ROSPH.
IF (R.LT.ROGAUS), THE CHARGE DENSITY IS SPHERICALY SYMMETRIC.
ITS FOURIER COEFFICIENTS ARE OBTAINED BY FILON'S RULE AT NRPWT
POINTS.
IF (ROGAUS.LT.R.LE.ROSPH), THE CHARGE DENSITY IS EXPANDED IN CUBIC
HARMONICS.
THE EXPANSION COEFFICIENTS ARE OBTAINED FROM CHARGE DENSITY ALONG
(DIRX,DIRY,DIRZ) DIRECTIONS.
THE FOURIER COEFFICIENTS OF THE EXCHANGE POTENTIAL ARE OBTAINED
BY THE FILON'S INTEGRATION METHOD BASED ON NFDL PCIN Points BETWEEN
TWO SPHERES.
THE CONTRIBUTIONS FROM REGION BETWEEN NEIGHBORING SPHERES ARE AS
FOLLOWS:
THE REGION IS DIVIDED INTO CUBES OF LENGTH A/(2*IECILD).
DENSITY**1/3 IS EXTRAPOLATED LINEARLY INSIDE EACH CUBE WHEN
THE FOURIER COEFFICIENTS ARE EVALUATED.
IF (IGRLV.EQ.0) THE CHARGE DENSITY IS APPROXIMATED BY ITS
SPHERICAL AVERAGE AND IS INTEGRATED UP TO THE RADIUS OF THE HIGHER
SEITZ SPHERE.

EXP(I K R) = ((N*PI**L*JL(K*R)*KLB(R) = KLB(R), R=-L,L), L=0, INFINITE)
JL(KR) IS THE SPHERICAL BESSEL FUNCTION OF ORDER L.
KLB(R) IS THE CUBIC HARMONIC OF ORDER L TYPE R.
DIMENSION RESTRICTIONS.

AXDAXIDIM, AY(AIDIM), AZ(AZDIM), MPW(1,1,1) WHERE I.EQ.IBCLND+2.
SIMP(J,K), COSINE(J,K) WHERE J.GE.IBCLND+1, K.GE.SQRT(MAXK)+2.
IMX(N), IMY(N), IMZ(N), ITP(6,M), WT(M), WHERE M=NO OF INDEPENDENT
POUNTS IN 1/48TH OF THE UNIT CELL GENERATED BY IBCLND.
RHOF(L*N) WHERE L IS NO OF POINTS INVOLVED IN CALCULATING THE
GRADIENTS.

NEW FEATURES

IVACR=2, IW=1, IDO=2: GET V(K) ONLY
IVACR=2, IW=2, IDO=1 OR 2: GET W(K) ONLY

IMPLICIT REAL*8(A-H, I-Z)
INTEGER*2 KX(8000), KX(8000), KX(8000), KX(8000), KB(8000), KB(8000), KB(8000)
INTEGER*2 MPW(34,34,34), IBT(6,1785), IAB(1785), IGR(1785), IAB(1785)
DIMENSION SIMP(33,100), CSPIN(33,100)
DIMENSION RHOB(14000), W(1785), IBOR(1505)
DIMENSION ARC(36), BCO(9), CBO(9), PBQ(4)
DIMENSION AX(500), AT(500), AZ(500)
DIMENSION R(201), ROH(1001), RIQ(201), FIEOR(7236), RWSIZ(101),
6WSOBR(8009)
DIMENSION SQ(8000)
COMMON/KBR, /CHGR, /CHGRD, /CHGRF, /CHGRG, /CHGRH, /CHGRK, /CHGRH
COMMON/CONF/CONF, /CONF, /CONF, /CONF, /CONF, /CONF, /CONF, /CONF, /CONF
& /CONF
COMMON/KR, /KBR, /KBR, /KBR, /KBR, /KBR, /KBR, /KBR, /KBR
COMMON/_EXPR/EXPR, /EXPR, /EXPR, /EXPR, /EXPR, /EXPR, /EXPR, /EXPR, /EXPR
& /EXPR
COMMON/LC/LC, /LC, /LC, /LC, /LC, /LC, /LC, /LC, /LC
COMMON/LOC/LOC, /LOC, /LOC, /LOC, /LOC, /LOC, /LOC, /LOC, /LOC
COMMON/TOT/TOT, /TOT, /TOT, /TOT, /TOT, /TOT, /TOT, /TOT, /TOT
EQUALITY/PER(1), /MPW(1,1,1)
PL=3.141592653589793
OMLTD=1.0/3.0
TWINH=2.0/3.0
FACTO(1)=1.0
DO 10 I=2,10
10 FACTO(I)=FACTO(I-1)*DFLOAT(I)

A=LATTICE CONSTANT (IN A. U. )
RADIUS= RADIUS OF THE SMALLER SPHERE.

READ(5,20) A, RADIUS
20 IOAMAT(IS10.5)
C

C V E K S U M = O .D O
C V C K P S N = O .D O
C V X C P S M = O .D O
C N P U P S H *O .D O
C N P D N S M = O .D O
C N P U D S H * O .D O
C N X C P S B = O .D O
C C  S C  ID C U B S1, B C C  ID CU B=2, F C C  ID C U B *4
C C IDIB IS T H E  N U M B E R  O F  T H E  D.L.V. <AI,AI,AZ)
C C IF (ISOBT.HE.0) B.L.V. IS S C B T E D  IN O B D E L E R  O F  IN C B E A S IN G  M A G N IT U D E .
C C IRC ELD *D IV ISIO N  IN T H E  U N IT  C E L L .
C C H B P N T *  DIVISION F O B  O.IE.B.LE.ROGAUS.
C C R P IL C N  DIVISION F O B  BOGAUS.IE.B.IE.BCSPH (R A D IU S  O F  JU ST T O U C H IN G
C C SPHERE).
C C IVXCB=0,NO C A L C U L A T IO N  O F  N  (K S ) F O B  T H E  T O T A L  E N E R G Y  A N D  X -A L P H A
C C P O T E N T IA L  U S E D  O N L Y .
C C IVXCB=1,CALCULATE VXC(KS) AND W(KS),USING X-ALPHA POTENTIAL.
C C IVXCB=2,CALCULATE VXC(KS) AND W(KS),USING VB POTENTIAL.
C
C============================================================================

C READ(5,30) IDCUG,NKPT,MAXK,MAX1,MAX2,NSM1,NSM2,NSM3,ISYM,IGRLY0,ISCT,
C IPUN,IRCEL,D,RFNLN,NNPNI,NGSIZ,IGAUS
C READ(5,30) IVXCB,JW,ICD

30 FORMAT(1615)
1RCM=IRCEL+2
DO 32 J=1,1RCM
DO 32 K=1,1RCM
32 MFP(K,J,K)=0
AAA=A*A*A
AKR=2.0*D*P1/4
AKR2=A*K*A
OMEGA=A/A/D/DPLOAT(IDCUB)
AHALF=A/2.0
COR=AHALF/DPLOAT(IRCEL)
40 FORMAT(2X,A8,215,8F7.4)
50 FORMAT(5F7.6)
60 FORMAT(1X,"EIP=".F20.6,3X,"COEF=".F16.6)
70 FORMAT(1X,"NC SP ".,I1,16.5X,"NC OF ORBITALS=".,16.5X,"ELECTRONS UP=".,
&8.3,5X,"ELECTRONS DOWN=".,F8.3,5X,"TOTAL ELECTRONS=".F8.3,/)
DSN=PBBAGA.DIOLA,FCOF

110 AX(I)=KKX(I)
AY(I)=KRY(I)
DIBX(I)=AX(2)
DIBY(I)=AY(2)
DIBZ(I)=AZ(2)

IF(NDIBC.EQ.1) GO TO 170
IST=3
DO 160 ND=2,NDIBC
NSD=ND-1
ISCL=IST
DO 150 I=ISCL,NDIBC
DO 140 ID=1,NSD
IF(AY(I)*DIBZ(ID)-AZ(I)*DIRZ(ID).EQ.0.0.AND.
&AZ(I)*DIBX(ID)-AX(I)*DIRX(ID).EQ.0.0.AND.
&AX(I)*DIBY(ID)-AY(I)*DIRY(ID).EQ.0.0) GO TO 150
140 CONTINUE
DIBX(ND)=AX(I)
DIBY(ND)=AY(I)
DIBZ(ND)=AZ(I)
IST=IST+1
IF(IST.LE.IDIRC) GO TO 160
150 CONTINUE
12=12+5
GO TO 120
160 CONTINUE
170 CONTINUE
180 CONTINUE

C GENERATE PERMUTED DIRECT LATTICE VECTORS
C
CALL GPEBKR(KKX,KKY,KKZ,KSCL,ISDIR,IEC,MAXR2,1,0)
IF(IECUC2.EQ.1) AHALF=1
DO 190 II=1,1DIM
AX(II)=AHALF*KKX(II)
AY(II)=AHALF*KKY(II)
190 AZ(II)=AHALF*KKZ(II)
CO=1.ELECT*PI/8.DO/CMEGA
FACT=1.DO/ORBSG
CNCO=1.DO/DSQRT(4.DO*EI)
BN04=1.25DO*DSQRT(21.DO)
BN05=231.DO/DSQRT(26.DO)/8.DO
BN08=65.DO/DSQRT(561.DO)/16.DO
CNCO=BN04*CN001
CN06=BN05*CN001
CN08=BN08*CN001
SIFPI=-6.DO*(3.DO/(4.DO*PI))**0.5THD
CDENS=4.DO*PI/ORBSG*CN001
CZFE=CDENS
CZFA=CZFE
CZWD=2.DO*PI/ORBSG
NZ=INCLUD+1
NDIRC=MNAND*NDIRC

C GENERATE OR READ IN THE PARAMETERS IN THE Ewald TYPE POTENTIAL.
C V(R)=-(2*Z+ALPHA)*EXP(-BETA1*R**2)/R+ALPHA*EXP(-BETA2*R**2)/R
C IF(EWALD.EQ.0) THE PARAMETERS ARE GENERATED IN SUBEXECUTE OPEWAD.
DSN=PHEAGA.DIOLA.FCOF

READ(5,200)IREWALD,ALPHA,BETA1,BETA2
200 FORMAT(110,3F15.4)
  N2= (AX (2) * AX (2) * AY (2) * AY (2) * AZ (2) * AZ (2) ) / 4.0
  CALL OPENAD(ALPHA,BETA1,BETA2,B2,5.0-1,2.0-1,50)
  GO TO 102
210 CONTINUE
  VPT1= (2.0 * ELECT * ALPHA) * DEXP (-BETA1*B2) / DSQRT (B2)
  VPT2=ALPHA * DEXP (-BETA2*B2) / DSQRT (B2)
  WRITE (6,101)IREWALD,ALPHA,BETA1,BETA2,VPTST
101 FORMAT (/,'2X,'2X, 'IREWALD=',I10,','ALPHA=',F15.4,'BETA1=',F15.4,
       'BETA2=',F15.4,'V=P15.4,'00(12,E20.5,/) )
102 CONTINUE
  IF (IG510.EQ.0) GO TO 300
C C
DEFINE EQUALLY SPACED POINTS IN 1/4TH OF THE UNIT CELL.
C CALL GEZPT(KKX,KKY,KKZ,ROHF,E,M,SUMW,1,0,1)
C MODIFY THE WEIGHTING FACTOR FOR THE CUBES THAT ARE INTERCEPTED BY
C THE SPHERE.
C CALL SPFHT(KKX,KKY,KKZ,ROHF,E,M,SUMW,1,0,1)
HFTIN=BSPHT
WRITE (6,600)A,BO,ELECT,EMAG,IDCUB,MMFT,MAKX,MAKY,MAKZ,ITNR,RHTIN,RFPTIN
600 FORMAT(/,'2X,'2X, 'A=',F15.4,'BO=',E15.4,'ELECT=',E15.4,'EMAG=',E15.4,'M1=',I5,
       'M2=',I5,'M3=',I5,'ITNR=',I5,'RFTIN=',E15.4,'RFPTIN=',E15.4,/) IF (IGAMNE.EQ.0) GO TO 300
C BOHF=BO/2.0
C SELECT POINTS THAT ARE INVOLVED IN CALCULATING THE GRADIENTS.
C J=0
DO 230 I=1,NSPHT
  RX=BOHF*KKX(I)+CBOHF+COB
  RY=COB*KKY(I)+CBOHF+COB
  RZ=COB*KKZ(I)+CBOHF+COB
  IF (RX+RY+RZ.LT.BOSPH) GO TO 220
  J=J+1
230 CONTINUE
  NB(I)=J
  GO TO 240
220 NB(I)=0
230 CONTINUE
  HFTIN=J
  J=0
250 CONTINUE
  IF (NB(I).EQ.0) GO TO 240
  J=J+1
  GO TO 250
240 CONTINUE
  KX(J)=KKX(I)
  KY(J)=KKY(I)
  KZ(J)=KKZ(I)
  WT(J)=RHCBHF(I)
260 CONTINUE
IDV1=I+1
CALL GADPT(NP,IX,IRY,IBZ,IBR,IDV1,NSINF,IDC)
KK=SQRT(FLOAT(MAXK2)) +2
BK=0
DO 270 I=1,III
SINE(I,1)=0.D0
270 COSINE(I,1)=1.D0
BK=0.D0
DO 280 K=2,KK
BK=BK+AKR
AK=AK*CORHAP
SINE(I,K)=0.D0
280 COSINE(I,K)=DSIN(AK)/AK
BK=0.D0
DO 290 K=2,KK
BK=BK+AKR
AK=AK*CORHAP
SINE(I,K)=DSIN(AK)/AK
CDIA=(DCOS(AK)-SIA)/(4.DO*AK)
RA=0.D0
DO 290 I=1,III
RA=RA+COR
RANK=RA*BK
SINE(I,K)=DSIN(RANK)*CCA
290 COSINE(I,K)=DCOS(RANK)*SIA
CMTIN=1.DO/(SUM*CDENS*6.DO)
300 CONTINUE
C IF IW=2,VCXCS1 IS USED TO CALCULATE W(BS)
305 READ(5,30,EN=610)KST,KEND,PKHCR,IBRIV,IKPTPB
307 CONTINUE
C CALCULATE THE CHARGE DENSITY.
C
310 CONTINUE
DGAUS=ROGAUS/DFLOAT(NRPWT-1)
RF=0.DO
DO 3201 =1,NRPWI
R(1)=RF
RF=RF+DGAUS
320 CONTINUE
CALL POE1C(AX,AY,AZ,IDIM,IBR1,IRY,IBZ,CCR,EPFI,CSINF,WT,WSF,IVXCH)
DPIFILN=(ROP3-ROGAUS)/DFLOAT(NCPIL-1)
RF=ROGAUS
DO 330 I=1,CPILON
CPILON(I)=RF
RF=RF+DPIFILN
330 CONTINUE
CALL POE1C(AX,AY,AZ,IDIM,CPILON,RFILON,PHRHCR,WDCB,HDIC,0,
6SFIW,IVXCH)
DGSZ=(ROWG3-ROPH)/DFLOAT(NWGSIZ-1)
RF=ROPH
DO 340 I=1,NWGSIZ
NWGSIZ(I)=RF
RF=RF+DGSZ
340 CONTINUE
U  U  U  uuuuu

£S N = P H B 1G A . E10LA . F C O F


3 * C H E C K D E N S , /

K 2 = - 1
DO 570 N P T = K S T , K E N D , K I N C M
IF (IG R I V . E C . 0) G O T O 410
K X = K X X (N P T)
K Y = K Y Y (N P T)
K Z = K K Z (N P T)
W B = B B (N P T)
K 2 = K S C (N P T)
G O T O 420
410 K 2 = N P T - 1
420 C O N T I N U E
IF (K 2 . N E . 0) G O T O 450

C

CALCULATE THE FOURIER COEFFICIENT V (K = 0)

K X = 0 . D O
C A L L F I L O I (C R O , 1 , N E P M T , B K , D B G A U S , B H O L , B , 0 , B R P M T , K I N D , C R I)
D O 425 I = 1 , B P T I N
IF (W T ( I ) . L E . 0 . D O ) G O T O 425
C O = 6 . D O * W T ( I )
II = I
C B 1 = C B 1 + R H O R V 1 ( I I ) * C O
II = II + B P T I N
425 C O N T I N U E

I F (I G R I V . E C . 0) G O T O 440
G U N W = E L E D N / O M E G A
G U N D W = E L E D N / O M E G A
D O 430 I = 1 , B P T I N
IF (W T ( I ) . L E . 0 . D O ) G O T O 430
C O = 6 . D O * W T ( I )
II = I
D O 429 K = 1 , K I N D
C B C ( K ) = C R O ( K ) + R H O R M P ( I I ) * C O
II = II + B P T I N
429 C O N T I N U E
430 C O N T I N U E
G O T O 550
440 C O N T I N U E
SUM = E L E C T / O M E G A
& C R I)
G O T O 460

C

CALCULATE THE FOURIER COEFFICIENTS ( K . G T . 0)

C

CALCULATE THE FOURIER COEFFICIENTS OF THE EXCHANGE POTENTIAL

450 C O N T I N U E
B K 2 = D F L O A T ( K 2)
B S = B K 2 * A K R 2
R K = D S Q E T ( B S)
I F (I G R I V . N E . 0) G O T O 480

C
DS=PHBAGA. DIOLA. FCOF

FOURIER COEFFICIENTS ARE GENERATED AS FUNCTION OF K**2.

CHARGE DENSITY**1/3 IS ASSUMED TO BE SPHERICALLY SYMMETRIC.

INTEGRATE FROM R=0 TO THE RADIUS OF THE WIGNER-SeIIZ SPHERE.

CALL FILON(CR0,1,NBPBT,BK,EBGAS,RHGB,R0,NBPBT,KIND)
CALL FILON(CRO,1,NFILDN,BK,DRFILN,PRHOR,RFILDW1,NFILDM,KIND)
CALL FILON(CRO,1,NWGSIZ,RK,DRWGSZ,NSRHOB,NWGSIZW1,NWGSIZ,KIND)

CALCULATE THE FOURIER COEFFICIENTS OF THE COULOMB POTENTIAL.

GET RO(K) UP AND SO(K) DN THEN V(K) FOR THE
COULOMB POTENTIAL

CALL CCDLOB(CHABO,P,SUBO,RS,FACT)
GUMUP=SUMP
IF(NSPIN.EQ.1) GC TO 451
CALL COULOM(CHABW,SUNDN,ES,FACT)
GUMD=SUMP
SUMP=SUMP+SUMP
GO TO 452

451 SUMP=2.DO*SUMP
GUM=SUMP

CONTINUE

GCOULAR=(SUM*8.DO*PI-COL)/ES
GCOUEL=SUM*8.DO*PI/RS
X=RS/(4.DO*BE1A2)
CALL CFHYF(1.DO,1.50DO,X,CFHYG,1.D-10)
EM=CFHYG*ALPHA/ETA1
X=RS/(4.DO*BE1A1)
CALL CFHYF(1.DO,1.50DO,X,CFHYG,1.D-10)
EM=EM+CFHYG*(-2.DO*ELECT-ALPHA)/ETA1
GEMLD=CHND*EM

460 CONTINUE

GUM=SUM
NWB=NWB
ANNB=DFLOAT(NNB)
IF(NSPIN.EQ.1) GC TO 470
BHK=CR0 (1)*C DEN9
GEXCH=CH0 (2)*CEXPA
GEXUP=CR3 (3)*CEXPE
GEXDN=CB0 (4)*CEXPE
IF(NPT.LE.KPTET.OR.(K2/200)*200.EQ.K2)
WRITE(6,580) K2,GCOUL,GEWLD,GEEX,GEIDP,GEIDN,SUM,PHOK
C
WHEN I1.EQ.1, GEXCH(KS)=VXC(KS)
C
WRITE(1) K2,GCOUL,GEWLD,GEEX,GEIDP,GEIDN
WRITE(10) K2,CUGOL,GEWLL,GEEX,GEIDP,GEIDC,GUMDF,GUNDF,GFU
VXKSON=VXKSON+GCOUEL
VXKPSM=VXKPSM+GCOUEL+SUM
VXKSUM=VXKSUM+GCOUL
VXKPSM=VXKPSM+GCOUL+SUM
IF(NPT.EQ.619.OR.(K2/500)*500.EQ.K2)
WRITE(6,640) VXKSON,VEKPSM,VXKPSM,VXKSUM,VEKPSM

CONTINUE

462 CONTINUE

464 FORMAT(65X,5F11.6)
FILE 2 IS USED FOR CALCULATION OF THE TOTAL ENERGY USING VEH

POTENTIAL ONLY

WHEN IN=EQ.2, GEICH(KS)=W(KS)

IF (IN.EQ.1) GO TO 570
WRITE (2) K2,GOOL,GEWLD,GEICH,GEUP,GEIDN
WRITE (11) K2,GOOL,GEWLD,GEICH,GEUP,GEWLD,GOOL
WPUPSM=WPUPSM+GEICH+SUMUP
WPDSM=WPDSM+GEIDN+SDDN
WPUPSM=WPUPSM+WPUPSM+WPDSM
WRITE (6,466) WPUPSM,WPDSM,WPUPSM,GO TO 570

466 FORMAT (76X,4F11.6)
470 CONTINUE
RHCK=CRU(1)*CDENS
GEICH=CRU(2)*CXEPE
IF (IN.EQ.2) GO TO 473
WRITE (1) K2,GOOL,GEWLD,GEICH
WRITE (10) K2,GOOL,GEWLD,GEICH,GOOL
CALCULATE SUMS OF VE(KS),VE(KS)*P(KS),VC(KS)*P(KS),VX(KS)*P(KS)

AND W(KS)*P(KS) FOR PAFARAG. ONLY
VEKSUM=VEKSUM+GOOUL
VEKPSM=VEKPSM+GOOUL+SUM
VCKSUM=VCCKSUM+GOOUL
VCCKSUM=VCCKSUM+GOOUL+SUM
VICPSM=VICPSM+GEICH+SUM
IF (NP.LE.KPTPTBA.EQ.(K2/200)*200.EQ.K2)
WRITE (6,475) K2,GOOUL,GEWLD,GEICH,GOOL,VEKSUM,VEKPSM,

473 CONTINUE
475 FORMAT (76X,15,1CP11.7)
477 FORMAT (76X,4F11.6)
490 FORMAT (76X,1F11.6)
497 CONTINUE
FOURIER COEFFICIENTS ARE GENERATED AS FUNCTION OF K VECTORS.

INTEGRATE FROM 0 TO HOGAUS.

IF (KS2.NE.K2) CALL FILLOW(BBC,1,MRPNI,NN,DRGHAUS,DRHOR,P,0,MRP1,KIND)
DO 490 K=1,KIND
490 FORMAT (BB0(K)
CALCULATE THE CONTRIBUTION FROM REGION BETWEEN NEIGHBORING SPHERES TO THE EXCHANGE POTENTIAL.

M1=KK+1
M2=KK+1
DO 510 IR=1,BPTIN
IF (I1(I3),LE,.LT.O,DO) GO TO 510
I1=IRX(I6)+1
I2=IRY(I8)+1
I3=IRZ(I6)+1
C1=COSINE(I1,N1)
C2=COSINE(I1,N2)
C3=COSINE(I1,N3)
C4=COSINE(I2,N1)
C5=COSINE(I2,N2)
C6=COSINE(I2,N3)
C7=COSINE(I3,N1)
C8=COSINE(I3,N2)
C9=COSINE(I3,N3)
S1=SINE(I1,N1)
S2=SINE(I1,N2)
S3=SINE(I1,N3)
S4=SINE(I2,N1)
S5=SINE(I2,N2)
S6=SINE(I2,N3)
S7=SINE(I3,N1)
S8=SINE(I3,N2)
S9=SINE(I3,N3)
C0=(C1*(C5*C9+C6*C8)+C2*(C4*C9+C6*C7)+C3*(C4*C8+C5*C7))*WT(IE)
D1=(S1*(C5*C9+C6*C8)+S2*(C4*C9+C6*C7)+S3*(C4*C8+C5*C7))*WT(IE)
D2=(S4*(C2*C9+C3*C8)+S5*(C1*C9+C3*C7)+S6*(C1*C8+C2*C7))*WT(IE)
D3=(S7*(C2*C9+C3*C5)+S8*(C1*C6+C3*C4)+S9*(C1*C5+C2*C4))*WT(IE)
I1P=IPT(1,IB)
I1M=IPT(2,IR)
I1P=IPT(3,IR)
I1M=IPT(4,IR)
I2F=IPT(5,IR)
I2M=IPT(6,IR)
I1=IE
DO 500 K=1,KIND
CBO(K)=CBO(K)+CO*HORBF(I1)*D1*(HORBF(I1P)-HORBF(I1M))
+D2*(HORBF(I2P)-HORBF(I2M))+D3*(HORBF(I3P)-HORBF(I3M))
I2=I2+1
I3=I1+1
I4=I2+1
I3=I3+1
I4=I4+1
I5=I5+1
I6=I6+1
I7=I7+1
I8=I8+1
I9=I9+1
I10=I10+1
I11=I11+1
I12=I12+1
C1=I12+1
C2=I12+1
C3=I12+1
C4=I12+1
C5=I12+1
C6=I12+1
C7=I12+1
C8=I12+1
C9=I12+1
S1=I12+1
S2=I12+1
S3=I12+1
S4=I12+1
S5=I12+1
S6=I12+1
S7=I12+1
S8=I12+1
S9=I12+1
I1=I1+1
I2=I2+1
I3=I3+1
I4=I4+1
I5=I5+1
I6=I6+1
I7=I7+1
I8=I8+1
I9=I9+1
I10=I10+1
I11=I11+1
I12=I12+1
I1=I1+1
I2=I2+1
I3=I3+1
I4=I4+1
I5=I5+1
I6=I6+1
I7=I7+1
I8=I8+1
I9=I9+1
I10=I10+1
I11=I11+1
I12=I12+1
500 CONTINUE
510 CONTINUE
C
C INTEGRATE FROM ROGALUS TO THE RADIUS OF TOUCHING SPHERE AND SUM
C OVER THE KUBIC HARMONIC EXPANSION.
C
1F (KS2.KZ.K1)

call fillon(ARO,MC1,MC2,BR1,0,6K,DRFILN,FLBGE,RFILW,0,6WFLDIN,KIND)
RKX=ARK*KK
RKY=ARK*KK
BKZ=ARK*KK
K2=(RKX/RK)**2
Y2=(RKY/RK)**2
DO 520 ND=1,NDINC
II=ND
DO 520 K=1,KIND
CBO(K)=CBO(K)+AKO(II)*CUBIC(ND)
II=II+NDINC

520 CONTINUE

C
C CALCULATE THE FOURIER COEFFICIENTS OF THE CHARGE DENSITIES FOR
C BOTH SPINS.
C
IF(KS2.EQ.K2) GO TO 540
KS2=K2
X=-BS/(4.DO*3ETA2)
CALL CPHIGF(1,DO,1.5DO,X,CFHYG,1.D-10)
ZH=CFHYG*ALPHA/BETA2
X=-BS/(4.DO*3ETA1)
CALL CPHIGF(1,DO,1.5DO,X,CFHYG,1.D-10)
ZH=ZH+CFHYG*(-2.DO*ELECT-ALPHA)/BETA1
GEMD=GMD*EW
CALL CCOULM(CHABUP,SUMUP,RS,FACT)
GUMDN=SUMDN
IF(NSPIN.EQ.1) GO TO 530
CALL CCOULM(CHABMN,SURMN,RS,FACT)
GUMDN=SUMDN
GCOUL=(SUMUP+SUBDN)*8.DO*PI-CC1)/RS
GCOUEL=(SUMUP+SUBDN)*8.DO*PI/RS
GO TO 540

530 GUMDN=GUMUP
GCOU=(2.DO*50 MOD*8.DO*PI-CC1)/RS
GCOUEL=2.DO*SUMUP*8.DO*PI/RS
GO TO 540

540 CONTINUE

550 CONTINUE
IF(KSPIN.EQ.1) GO TO 560
RMOK=CBO(1)*CDENS
GEXCH=CBO(2)*CEXFA
GEXUP=CBO(3)*CEXFE
GEXDN=CBO(4)*CEXFE
GDSFA=CBO(5)*CEXFE
GDSUP=CBO(6)*CEXFE
GDSDN=CBO(7)*CEXFE
GDSUD=CBO(8)*CEXFE
GDSUL=CBO(9)*CEXFE
MNNB=NNB
ANAB=DFLCAT(JNNB)
DSM=P8SAGA_SIOLA_FCOF

1* F7.2,3X* MAG Mo='F7.4,3X* IDCUB='F7.4,3X* 2*K Mo='I5.3X* K2 MAX='I5.3X* P Mo='I6.3X* P2 MAX='I5.3X* ORBIT
3*LS Mo='I5.3X* LS* GEN HL='I2.3X* SORT='I2.3X/'I1X* R DIV='I5.3X
4* R PTS='I5.3X* NONSHELLRICAL PTS='I5.3X* GAUS PTS='I5.3X
6* DIRECTION='I5.3X* MXFLN='I6.3X* NWGSI='I5.3X

IF (IN.EQ.2) GO TO 603
END FILE 1
IF (IVXCH.EQ.2) IN=IN+IDO
IF (IN.EQ.2) GO TO 307
GO TO 300

603 CONTINUE
END FILE 2
GO TO 300

610 STOP
END

SUBROUTINE VXCS1(UP,DN,DENS,EXPA,EXUP,EXDN,DVDBR,DVDRM,DVDDB,1DWDDB,DVPDR,DVDRH,DVDRN,DVDUM,DVDMN,DEL0,DVT,DVTA)

C REVISION OF SUBROUTINE EXBATH, DECEMBER 1979

IMPLICIT REAL*8(A-H,C-Z)

C COMMON/TOTLE/IV

F(2) = (1.0D0+Z*3)**DLOU (1.0D0+1.0D0/2)*Z/2.0D0-Z-Z-1.0D0/3.0D0

DENS=DF+D0

PI=3.141592653589793D0

ON THE=1.0D0/3.0D0

AA=1.0D0/2.0D0*ONETHD

CCF=4.0D0*AA/(3.0D0*{1.0D0-AA})

ONETHD=1.0D0/4.0D0

FORTHD=4.0D0/3.0D0

CP=0.04612D0

BP=39.7D0

CF=0.02628D0

BF=70.4D0

B=3.0D0/(4.0D0*PI*DENS)**ONETHD

UPX=2.0D0*(9.0D0*PI/4.0D0)**ONETHD/(FI*RS)

ECP=-CF*FS/FP

ECF=CF*FS/BS

UNL=COEF*(ECF-ECP)

UCF=CP*DLOG(1.0D0+BP/RS)

UPH=1.0D0/4.0D0

aaa=UPH+UNC

TC=UCF-UCP-FORTHD*(ECF-ECP)

BP=(UCP-AAA;/UCF)/(1.0D0-AA)

C=TC/(1.0D0-AA)

UXP=UP/DENS

XD=DN/DENS

IF (IN.EQ.2) GO TO 10

X4=UXP*FORTHD+XD**FGTHD

C=BC*X4

Q=2.0D0*UXP)**ONETHD

QB=2.0D0*XD)**ONETHD

QC=AA*QA

QD=AA*CB

EXUP=QC*AA*QA

EXDN=QC*AA*QB

EXPA=A+B+AA*E

FLX=(X4-AA)/{1.0D0-AA}

DVT=28.0D0*ONETHD*(ICF-ICP-6.0D0*(UCF-UCP)/7.0D0)*{FI+AA/1.0D0-AA)

DV1 = DVT-CF*FLX/(FL+IS)-CP*FP{1.0D0-FLX/(FP+IS)
DSN=PBBAGA.DIOLA.FCOF

DVT=OMEHID*DVT/DENS
DVUDR=DVT*OEHID*AA/CF*DF+6.DO*OEHID*QC/DENS
LYNDR=DVT+OEHID*QB/AB+6.DO*OEHID*CD/DENS
DVUDEN=DVT+RJHID*QC*(QC+CD)/DENS
DVUDNR=DVUDRU
DVPADE=DVT+8.DO*OEHID*AA/DENS+OEHID*QC/DENS
DVUDRH=0.5DO*(DVUDRU+DVUDRN)
DVUDRN=0.5DO*(DVUDRU+DVUDRN)
DVNDR=0.5DO*(DVUDRN-DVUDRN)
DL0=0.5DO*(DVUDRH+DVUDNR)
DL1=0.5DO*(DVUDRH-DVUDNR)
DL2=0.5DO*(DVUDRN-DVUDRN)

RETURN

10 CONTINUE
GR=AA*(DCF-CUP-7.DO*OEHID*(ECF-ECP))/(1.DO-AA)
PH=(OEPF*UPX+UAC+GB)/AA
GR=DCF-ECP-UAC-GB
WUP=PE*XUP*OEHID*GB
WE=DF*XHM*OEHID*GB
MNP=PR*AA+GB
DQDRS=AA*(CF*RF/(RS*RF)-CF*RF/(RS*RF)-7.DO*(ECF-ECP-UAC-UAC))/
(1.DO-AA)/BS
DQDRS=UPX/(4.DO*AA*GB)+4.DO*(ECF-ECP-UAC-UAC)/(1.DO-AA)/BS+
(1.DO-AA)/BS
DQDRS=CF*RF/ES/(RS*RF)-3.DO*(ECF-ECP-UAC-UAC)/BS+4.DO*AA*(ECF-ECP-UAC-UAC)

END

SUBROUTINE POEIC1(AX,AY,AZ,IDLIN,NBPMT,R,RHOR,WEIRC,MDTOL,IGNAT,
CNSFIN,IVXCH)

C
CALCULATE THE KUBIC HARMONICS EXPANSION COEFFICIENTS OF THE
C FUNCTIONS OF THE CHARGE DENSITIES.
C GAUSSIAN TYPE ORBITALS ARE USED.
C
IMPLICIT REAL*8(A-F,H,O-Z)
DIMENSION AX(IDLIN),AY(IDLIN),AZ(IDLB),BHCC(1),R(1)
DIMENSION CC(4,4),C(4)
COMMON/XYK/(7,14),EX(7,14),FACTO(10),LB(7),NOBB(7),KSTA
C C CALCULATE THE KUBIC HARMONICS ALONG EACH DIRECTIONS.

SIXPA=SIXPI/2. DO**ONETHD * 
CONST=1.D0/(4.D0*PI)
IF (IGNAT.EQ.0) GO TO 50
DO 101=1,NDTOL
EB=EX(I) *Bx(I) *BY(I) +BZ(I) *BZ(I)
EB=DSGRT(ER)
BY(I) =BY(I) /BA
BZ(I) =BZ(I) /BA
X2=EX(I) *Bx(I)
Y2=BY(I) *BY(I)
Z2=EZ(I) *BZ(I)
X4=X2*X2
Y4=Y2*Y2
Z4=Z2*Z2
C4t=X4+Y4+Z4-0.6D0
C61=X2*Y2+2.*C41/22. DO-1.D0/105. D0
C61=X4*X4+Y4*Y4+Z4*Z4-5.6D0*C61-210. D0*C41/143. D0-1.D0/3. D0
C61=CN061
C81=X2*Y2*Z2+C41/CNC41
ALBAGE (6,60) EX(I),BY(I),BZ(I), (CMAT(I,J),J=1,NDTOL)
CONTINUE
C C CALCULATE THE INVERSE OF THE MATRIX.

CALL CMS(MNTOL,CMAT,CC,D,DEI,4)
DO 201=1,NDTOL
20 WHITE(6,30) RX(I),BY(I),BZ(I), (CMAT(I,J),J=1,NDTOL)
30 PFORMAT(1X,'A',13F10.5) ,14X,'KDB1 C HAB A . COEF. P THE P
40 PFORMAT(1X,'F15.5') ,14X,'KDB1 . KUBIC H AEM. COE. F OR THE P
50 CONTINUE
C C CALCULATE THE DENSITY ALONG EACH DIRECTIONS (BY(I),BY(I),BZ(I))

AND THE KUBIC HARMONIC EXPANSION COEFFICIENTS.

WHITE(6,60)
60 PFORMAT(1X,'A',14X,'DENSIT',10X,'KUBIC H AEM. COE. F OR THE P
70 CONTINUE
C C FERROMAGNETIC

1KKTOL=1KHTOL=9
DO 70 I=1,1KKTOL
70 BHK(I)=0.D0
DO 160 KB=1,1KHTOL
DEPST=0.D0

DSN=PHYGAD.IO.LA1.FCOF

540 CONTINUE
130 CONTINUE
140 CONTINUE
DENS=RHRB(KR)*CM001
WRITE(6,150)KR,EB(KR),DENS,CX,UP,DN,LO,D1,D2,D3,D4,DU,DU
150 FORMAT(1X,1A,F7.3,9(1X,E10.4),2(1X,E9.3))
160 CONTINUE
RETURN
170 CONTINUE

C PARAMAGNETIC.

180 BHRB(I)=0.DO
DO 270 KR=1,NBINT
DO 250 MD=1,NDTCL
DENSUP=0.DO
X=R(KR)*RX(ND)
Y=R(KR)*RY(ND)
Z=R(KR)*RZ(ND)
DO 230=1,NDSTA
180 CONTINUE
GO TO 190
190 SUM=0.DO
DO 220 JO=1,IDIM
PSI=0.DO
BA2={(AX(JJ)-X)**2+(AY(JJ)-Y)**2+(AZ(JJ)-Z)**2}
HA=DSQRT(BA2)
IF(HA.LE.0.0) GO TO 200
DO 190 J=1,N
BA=X*X+Y*Y+Z*Z
IF(BA.GT.25.0) GO TO 190
BEX=C(J,0)*RA**IEB*EXP(-BA*
PSI=PSI+BEX
190 CONTINUE
GO TO 220
200 IF(XB.WX.0) GO TO 220
DO 210=1,N
PSI=PSI+C(J,0)
210 CONTINUE
220 SUMP=SUM+PSI*PSI
DENSUP=DENSUP+SUM*CHARO(I)*CONST
230 CONTINUE
IF(IVXCB.EQ.2) GO TO 233
DENS=DENSUP**2.DO
UP=DENSUP**ONIMTH*SIXP1
GO=DENS**TWTHY*SIXPA/3.DO
GO TO 237
233 CALL VCCBS1(DENSUP,DENSUP,DENS,CX,UP,DN,D1,D2,D3,D4,DJ,CB,CE,CF,DE10,DEL1,DEL2)
237 CONTINUE
DO 240 I=1,NK16
IKR=(I-1)*MRPHT+NR
12=IKR+IKRT
13=12+IKRT
BHRB(IKR)=EHOM(IKR)*CMAT(I,ND)*DENS
BHRB(I)=BHRB(I)+CMAT(I,ND)*UP
P5=PA+1(C1).J  
DO 40 1=1,7
  30 IF(EBEM.W<0.GC 10 50  
  20 CONTINUE
  30 CONTINUE
P5=PA+1(EX.G2,7ZD.GC 10 20  
  10 A=EF.X=EX.G2,7ZD.GC 10 20  
  20 CONTINUE
  10 CONTINUE
  20 CONTINUE
  30 CONTINUE
V=V2.00  
DO 50 2=1,10  
  40 IF(EBX.W<0.GC 10 50  
  30 CONTINUE
  40 CONTINUE
  30 CONTINUE
V=V4.00  
DO 60 1=1,10
  50 IF(EBX.W<0.GC 10 50  
  40 CONTINUE
  50 CONTINUE
  40 CONTINUE
V=V6.00  
DO 70 1=1,10
  60 IF(EBX.W<0.GC 10 50  
  50 CONTINUE
  60 CONTINUE
  50 CONTINUE
V=V8.00  
DO 80 1=1,10
  70 IF(EBX.W<0.GC 10 50  
  60 CONTINUE
  70 CONTINUE
  60 CONTINUE
V=V10.00  
DO 90 1=1,10
  80 IF(EBX.W<0.GC 10 50  
  70 CONTINUE
  80 CONTINUE
  70 CONTINUE
V=V12.00  
DO 100 1=1,10
  90 IF(EBX.W<0.GC 10 50  
  80 CONTINUE
  90 CONTINUE
  80 CONTINUE
V=V14.00  
DO 110 1=1,10
 100 IF(EBX.W<0.GC 10 50  
  90 CONTINUE
100 CONTINUE
  90 CONTINUE
V=V16.00  
DO 120 1=1,10
 110 IF(EBX.W<0.GC 10 50  
 100 CONTINUE
110 CONTINUE
 100 CONTINUE
40 CONTINUE
50 SUM=SUM+PSI*PSI
   DRUP=SUM*CHAR(I)*CONST
   DRDN=SUM*CHARN(I)*CONST
   DENSUP=DENSUP+DRUP
   DEWSDN=DEWSDN+DRDN
   IF (IGAU. NE.0) GO TO 60
   DEF=DRUP+DRDN
   WRITE (6,70) DEF,DEWSUP,DEWSDN,
60 CONTINUE
70 FORMAT (41X,3F20.5,15)
   DENS=DENSUP+DEWSDN
   IF (IGAU. NE.0) WRITE (6,90) R2,X,Y,Z,ENS,DENSUP,DENSDN,WT(KB)
   IF (IFUN. NE.0) WRITE (7,80) X,Y,Z,DENS,DENSUP,DENSDN,WT(KB)
90 FORMAT (3F9.7,1X,4F13.7)
   CONTINUE
   FORMAT(1X,4F10.5,4X0.6,15)
   IF (IGAU. NE.0) GO TO 93
   CX=DENS**ONESS*SIPI
   DN=DENSDN**ONEID*SIPI
   DO=DENS**TWTHI*SIPI/3.D0
   LI=DENSUP**TWTHI*SIPI/3.D0
   D2=DENSDN**TWTHI*SIPI/3.D0
   GO TO 97
93 CALL VCBVS1(DENSUP,DEWSDN,DENS,CI,OP,DN,D1,D2,D3,D4,D0,CA,CE,
                   &CP,DELO,DELI,DEL2)
97 CONTINUE
   BHOB1(KR)=CMFTIN*DENS*B2
   BHOB(KR)=CMFTIN*DENS
   BHOB(KR+MRPNT)=CMFTIN*CX
   BHOB(KR+2*MRPNT)=CMFTIN*DP
   BHOB(KR+3*MRPNT)=CMFTIN*DN
   BHOB(KR+4*MRPNT)=CMFTIN*D0
   BHOB(KR+5*MRPNT)=CMFTIN*LI
   BHOB(KR+6*MRPNT)=CMFTIN*D2
   BHOB(KR+7*MRPNT)=CMFTIN*D3
   BHOB(KR+8*MRPNT)=CMFTIN*D4
100 CONTINUE
RETURN
110 CONTINUE
C
C PARAMAGENTIC.
C
120 FORMAT (/6X,*R**,10X,**'X',10X,**Y',10X,**Z',18X,**'DENSITY',/)
   DO 190 KR=1,NRPMT
   DENSUP=0.D0
   X=IRX(KR)*COR
   Y=IRY(KR)*COR
   Z=IRZ(KR)*COR
   E2=X*X+Y*Y+Z*Z
   DO 1701=1,NSTA
   IBB=IB(I)-1
   SUM=0.D0
   M=MORE(I)
   DO 160 JJ=1,IDIM
   (text continues...)

---

107
DSN=PHDAGA.DIOLA.FCCP

10 CONTINUE
20 CONTINUE
   IF (R1K.1.1.D-5) GO TO 120
   TH=TH*TH
   HH=TH*TH
   IF (TH.1.1.D-4) GO TO 30
   SIN1=DSIN(TH)
   COS1=DCOS(TH)
   SIN2=2.D0*SIN1*COS1
   ALFA2=(1.D0+2.SIN2/(2.D0*TH)-2.D0*SIN1*SIN1/TH2)/TH
   BETA2=2.D0*((1+2.SIN1*COS1-SIN2/TH2)/TH2
   AGA=4.D0*(SIN1/TH-COS1)/TH2
   GO TO 40
30 CONTINUE
   TH=TH*TH
   HH=TH*TH
   ALFA2=2.D0*TH3*(1.D0/45.D0-TH2/315.D0+TH4/4725.D0)
40 CONTINUE
   IF (ND1C.EQ.1) GO TO 100
   DO 90 I=1,NWPNT
   R1K=KK*RPIION(I)
   CR0=1.D0/(R1K*BAR)
   CR1=3.D0/(R1K*BAR)
   CR2=DSSIN(BAR)/BAR
   CR3=DCOS(BAR)/BAR
   SPPS=CR2*RPIION(I)
   SP12=CR1*CR2=SPPS-3.D0*CR3/BK
   SPBN=SPPS
   IF (I.NE.1.AND.1.WE.NWPNT) GO TO 50
   APBELS=CR3*RPIION(I)
   TPBELS=APBELS
   TPBB2=DCBFLX(CR1*CR3-APBELS,-3.D0*CR2/BK)
   TPBR=TPBELS
50 DO 90 I=1,MDIRC
   IF (WD.I.I) GO TO 60
   C1=DFLCHR(2.0)
   C1=2.D0*CL-1.D0
   C3=C1-2.D0
   C5=C3-2.D0
   C6=4.D0*CL-6.D0
   SPBELS=(C3*C1-CH0-C6/C5)*SPBN2-C1/C5*SPBN4
   SPBN=SPPS
   SPBERT=SPBELS
   IF (I.NE.1.AND.1.WE.NWPNT) GO TO 60
   TPBELS=(C3*C1-CH0-C6/C5)*TPBR2-C1/C5*TPBN4
   TPBN=TPPS
   TPBR=TPBELS
60 CONTINUE
   IF ((I/I)*2.EQ.1) SPBELS=SPBELS*AGAMA
   IF ((I/I)*2.EQ.1) SPBELS=SPBELS*BETA
   IF (I.NE.1.AND.1.WE.NWPNT) GO TO 70
   EELS=TPBELS*(1.0,1.D0)
   IF (I.EQ.1) SPBELS=SPBELS/2.D0+ALPHA*BELS
   IF (I.EQ.1) SPBELS=SPBELS/2.D0+ALPHA*BELS
   IF (I.EQ.1) SPBELS=SPBELS/2.D0+ALPHA*BELS
70 CONTINUE
   SPEELS=SPBELS*DFILIN
DSN=PESAGA+DIOLA+FCOF

\[
\text{IND} = (\text{ND}-1) \times \text{NPMT} + 1
\]

\[
\text{AD} = \text{ND}
\]

\[
\text{DO} \ 80 \ \text{K} = 1, \text{ND}
\]

\[
\text{ARO} (\text{KD}) = \text{ARO} (\text{KD}) + \text{RHOR} (\text{IND}) \times \text{SPBELS}
\]

\[
\text{IND} = \text{ND} + \text{NDIM}
\]

\[
\text{KU} = \text{KD} + \text{KJRC}
\]

80 \text{ CONTINUE}

\[
\text{K} = \text{K} - 1
\]

\[
\text{CONTINUE}
\]

90 \text{ CONTINUE}

\[
\text{RETURN}
\]

100 \text{ CONTINUE}

\[
\text{DO} \ 110 \ I = 1, \text{NPMT}
\]

\[
\text{ER} = \text{KK} \times \text{RFLON} (1)
\]

\[
\text{SPBELS} = \text{DSIN} (\text{RAK}) \times \text{RFLON} (1) / \text{RB}
\]

\[
\text{IF} (I / 2) = 2 \times \text{KJ} - 1 \text{ SPBELS} = \text{SPEELS} \times \text{AGAMA}
\]

\[
\text{IF} (I / 2) = 2 \times \text{KJ} - 1 \text{ SPBELS} = \text{SPBELS} \times \text{BETA}
\]

\[
\text{IF} (I - \text{EQ} - 1) \text{ SPBELS} = \text{SPBELS} / 2 \times \text{DO} \times \text{AFLHA} \times \text{ECOS} (\text{RAK}) \times \text{RFLON} (1) / \text{RB}
\]

\[
\text{IF} (I - \text{EQ} - 1) \text{ SPBELS} = \text{SPBELS} / 2 \times \text{DO} - \text{AFLHA} \times \text{DCOS} (\text{RAK}) \times \text{RFLON} (1) / \text{RB}
\]

\[
\text{SPBELS} = \text{SPBELS} \times \text{DFILM}
\]

II = I

\[
\text{DO} \ 110 \ K = 1, \text{KIND}
\]

\[
\text{ARO} (\text{K}) = \text{ARO} (\text{K}) + \text{RHOR} (\text{II}) \times \text{SPBELS}
\]

II = II + \text{NDIM}

110 \text{ CONTINUE}

\[
\text{RETURN}
\]

120 \text{ CONTINUE}

\[
\text{K} = 0
\]

\[
\text{DO} \ 130 \ I = 1, \text{NPMT}, 4
\]

\[
\text{II} = I
\]

\[
\text{CO1} = \text{RFLON} (I) \times \text{DFILM} \times 14 \times \text{DO} / 45 \times \text{DO}
\]

\[
\text{IF} (I - \text{EQ} - 1) \text{ AND } I - \text{EQ} - \text{NPMT} \text{ CC1} = \text{CO1} \times 2 \times \text{DO}
\]

\[
\text{AR1} = \text{AR1} + \text{RHOR} (\text{II}) \times \text{CC1}
\]

\[
\text{CO} = \text{RFLON} (I) \times 2 \times \text{DFILM} \times 14 \times \text{DO} / 45 \times \text{DO}
\]

\[
\text{IF} (I - \text{EQ} - 1) \text{ AND } I - \text{EQ} - \text{NPMT} \text{ CO} = \text{CO} \times 2 \times \text{DO}
\]

\[
\text{DO} \ 130 \ K = 1, \text{KIND}
\]

\[
\text{ARO} (\text{K}) = \text{ARO} (\text{K}) + \text{RHOR} (\text{II}) \times \text{CO}
\]

II = II + \text{NDIM}

130 \text{ CONTINUE}

\[
\text{NP2} = \text{NPMT} - 2
\]

\[
\text{DO} \ 140 \ I = 3, \text{NP2}, 4
\]

\[
\text{II} = I
\]

\[
\text{CO1} = \text{RFLON} (I) \times \text{DFILM} \times 24 \times \text{DO} / 45 \times \text{DO}
\]

\[
\text{AR1} = \text{AR1} + \text{RHOR} (\text{II}) \times \text{CC1}
\]

\[
\text{CO} = \text{RFLON} (I) \times 2 \times \text{DFILM} \times 24 \times \text{DO} / 45 \times \text{DO}
\]

\[
\text{DO} \ 140 \ K = 1, \text{KIND}
\]

\[
\text{ARO} (\text{K}) = \text{ARO} (\text{K}) + \text{RHOR} (\text{II}) \times \text{CO}
\]

II = II + \text{NDIM}

140 \text{ CONTINUE}

\[
\text{NP3} = \text{NPMT} - 1
\]

\[
\text{DO} \ 150 \ I = 2, \text{NP3}, 2
\]

\[
\text{II} = I
\]

\[
\text{CO1} = \text{RFLON} (I) \times \text{DFILM} \times 64 \times \text{DO} / 45 \times \text{DO}
\]

\[
\text{AR1} = \text{AR1} + \text{RHOR} (\text{II}) \times \text{CO1}
\]

\[
\text{CO} = \text{RFLON} (I) \times 2 \times \text{DFILM} \times 64 \times \text{DO} / 45 \times \text{DO}
\]

\[
\text{DO} \ 150 \ K = 1, \text{KIND}
\]

\[
\text{ARO} (\text{K}) = \text{ARO} (\text{K}) + \text{RHOR} (\text{II}) \times \text{CO}
\]

II = II + \text{NDIM}
I l l
DSN-PBBAGA.CIOII.fCOF
IS O  COI N O E
B E T U B H
END
//LKED.SISL1B D O  DSN=D1103.CALLOA.HVCAPLIG.DIS=SHR
// DD DSN=D1103.CALLOA.BNDFKG_SUB11B.COMPL_DISP=SHR
// DD DSN=SYS1.VCPFLIG_DISP=SHR
// DD DSN=SYS2.POB11B,DISP=SHR
// DD DSN=SYS2.SSP.LIG,DISP=SHR
// DD DSN=SYS2.PLOT11.LID,DISP=SHR
//GO-F101F001 DD UNIT=3380, VOL=SER=USE177,DISP=(NEW,CATLG),
// SPACE=(TRK,(10,10),RLSE),
// DCB=(BLKSIZE=06404,RECFM=VBS,LBLCE=64),
// DSNNAME=PBBAQA.DICLA.FE5F84.BCC.VK1
//GO-F101F002 DD UNIT=3380, VOL=SER=USE177,DISP=(NEW,CATLG),
// SPACE=(TRK,(10,10),RLSE),
// DCB=(BLKSIZE=02804,RECFM=VBS,LBLCE=28),
// DSNNAME=PBBAQA.DICLA.FE5F84.BCC.VK2
//GO-F102F001 DD UNIT=3380, VOL=SER=USE177,DISP=(NEW,CATLG),
// SPACE=(TRK,(10,10),RLSE),
// DCB=(BLKSIZE=06404,RECFM=VBS,LBLCE=64),
// DSNNAME=PBBAQA.DICLA.FE5F84.BCC.VK3
//GO-F102F002 DD UNIT=3380, VOL=SER=USE177,DISP=(NEW,CATLG),
// SPACE=(TRK,(10,10),RLSE),
// DCB=(BLKSIZE=02804,RECFM=VBS,LBLCE=28),
// DSNNAME=PBBAQA.DICLA.FE5F84.BCC.VK4
//GO-F110F001 DD UNIT=3380, VOL=SER=USE177,DISP=(NEW,CATLG),
// SPACE=(TRK,(10,10),RLSE),
// DCB=(BLKSIZE=6600,RECFM=VBS,LBLCE=60),
// DSNNAME=PBBAQA.DICLA.FE5F84.BCC.VKL
//GO-F110F002 DD UNIT=3380, VOL=SER=USE177,DISP=(NEW,CATLG),
// SPACE=(TRK,(30,10),RLSE),
// DCB=(BLKSIZE=6600,RECFM=VBS,LBLCE=60),
// DSNNAME=PBBAQA.DICLA.FE5F84.BCC.VKL
//GO-SYSL DD *
5.4057 1.0
2 8000 20000 1.0 400 25 2 3 1 1 0 24 201 201 101 0
2 1 1 0
IRON 4 14 1.00 1.00 1.00 1.00 1.00 1.00 0.50 0.50
257539.000000 0.000290 -0.000900 0.000300 -0.000100
36636.900000 0.002260 -0.000680 0.000250 -0.000050
8991.440000 0.011520 -0.003540 0.001310 -0.000270
254.040000 0.005660 -0.001410 0.000520 -0.0001120
84.477000 0.043050 -0.046680 0.017380 -0.003660
312.527000 0.314220 -0.175350 0.045270 -0.009630
125.593000 0.408780 -0.219620 0.085050 -0.017940
53.498700 0.211630 -0.126610 0.058970 -0.012940
17.715100 0.017650 0.577710 -0.304220 0.068870
7.376770 0.002920 0.604690 -0.495030 0.114380
2.018670 0.000860 0.054560 0.671410 -0.192220
0.779935 0.000410 -0.009560 0.593010 -0.307100
0.114220 0.000110 0.002290 0.011490 0.579850
0.041889 -0.000050 -0.000100 -0.003120 0.558820
125.840000 0.002890 -0.000900
396.392000 0.020150 -0.091990
126.586000 0.091990 -0.034780
49.115600 0.259910 -0.101890
20.503500 0.428870 -0.183100
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```
APPENDIX A.2: New Version of PROGRAM SCF2

---

DSN=PHBAGA-DIOLA-SCF

---

//PHBAGA01 JCN (1103,60245,010,3), 'PH DIOLA', MSGCLASS=5, // NOTIFY=PHBAGA //AFTER PHBAGA00 //JOBPARM SHIFT=N //ROUTE PRINT PHYSICS // EXEC FORTHCLG,PARF.FCFT='NOSOURCE,LANGVL(66),OPT(2)', // PARM.LKED=N0XREF,REGION=1200K,TIME=999 //FORT.SYSIN DD *

---

PROGRAM SCF2

THE FIFTH PART (FERRCMAGNET) OF

A GENERAL PROGRAM TO CALCULATE SELF-CONSISTANT ENERGY BANDS

USING THE MODIFIED TIGHT BINDING OR LCGC METHOD

BY

C.S. WANG AND J. CALLAWAY

TOTAL ENERGY FEATURES

BY

J. CALLAWAY, X. ZOU, AND D. BAGAYOKC

DEPARTMENT OF PHYSICS

LOUISIANA STATE UNIVERSITY

BATON ROUGE LOUISIANA 70803

---

ROUTINES USED IN SCF2

C DIAGHS (FROM PROGRAM BND)
C DIGEN (FROM PROGRAM BND)
C DHTDS FROM IBM S.S.P. (NOT INCLUDED IN THIS PACKAGE)
C DHTDR FROM IBM S.S.P. (NOT INCLUDED IN THIS PACKAGE)
C FEBMIE (FROM PROGRAM SCF1)
C GBZPT (FROM FFCGBAH FCOF)
C GPERM (FROM PROGRAM FCOF)
C PUTMAT (FROM PROGRAM BND)
C SUMOKV (FROM FFCGBAH FCOF)
C TDBZPT (FROM PROGRAM SCF1)
C TDVL (FROM PROGRAM SCF1)
C TDELECT (FROM FFCGBAH FCOF)

---

COMMON BLOCKS OCCURRING IN SCF2

---

ROUTINES IN WHICH THEY ARE USED

C LCA SCF2
C LCB SCF2
DIMENSION RESTRICTIONS.
IPT(*,IPTOL) WHERE IPTOL IS THE NUMBER OF TETRAHEDRONS IN 1/48TH
OF THE BZ.
WKET, DIMENSION CF KEX,KEX,KBZ,WT
NK(1,1,1), L=2=SQR(K2MAX)+1
NKPS, DIMENSION OF KPENX,KPENY,KPENZ,KAGF,KSO,
NKPS=NUMBER OF INDEPENDENT R.L.V. WITH K**2.LE.4*K2MAX*1
NKPS, DIMENSION OF KSX,KSY,KSZ,KNR,ALAMUP,ALAMDN,ALARP
FUP(NBFERN,NE),EDN(NBFERM,NE),
RHIUP(NKPSRM,NKPSM,NKENPS),BUCDN(NKPSRM,NKPSM,NO),ZUP(NBFERN,
NKZPS)
EDN(NBFERN,NKZPS)
WTRIS=NB*(NP+1)/2, DIMENSION OF SIJ,HUP,HDM,OV
GKUP(NB),GIDM(NB),XUP(NB,NE),XDN(NB,NE)

** IMPLICIT REAL(A-H,O-Z)
** REAL*4 SIJ(0946)
INTEGER*2 IPT(4,500),KBX(140),KBY(140),KBZ(140),
ENK(24,24,24),KPENX(3JO),KPENY(3JO),KPENZ(3JO),KASIGP(3000)
INTEGER*2 KSX(900),KSY(900),K5Z(900),KNE(900),K52(900)
DSN=PHBAGA.DIOLA.SCF

DIMENSION KQDU(3000)
DIMENSION FUP(15,91),EDN(15,91),RHOUF(40,15,91),ALAMUP(900),
               DWDUPF(900),WIT(91)
DIMENSION FDN(15,91),EDN(15,91),RHODN(40,15,91),ALAMDN(900),
               DWDPDA(900),ALAMPA(900),DWDPDU(900),DWDPDA(900)
DIMENSION MUP(0946),OV(0946),XUP(43,43),GXUP(43)
DIMENSION EDN(0946),EDN(43,43),GDN(43)

THE FOLLOWING ARRAYS MUST BE DIMENSIONED AT LEAST NKPRT.

DIMENSION VK0(40),WUP(40),WDK0(40),WXUP0(40),CYKOD(40),CYKNW(40),
               1CIXUPW(40),DKU0(40),DKUPOD(40),DKUPOW(40),DKUP0(40), dvAKUP(40)
2,CI9UP0(40),OXUP(40)
DIMENSION DKNO(40),DKDND(40),DKDNO(40),DKDKNW(40),DKOKDN(40), dvAKDN(40)
1,CIXNOD(40),DVDN(40),VXNO(40),CXDNW(40)
COMMON/LCA/HUP,OV
COMMON/LCB/HODN
COMMON/SPACE/FUP,FDN

EQUIVALENCE(FUP(1,1),SLJ(1))
& (HUP(1),BHGFUP(1,1,1))
& (HDN(1),BHODN(1,1,1))
PI=3.141592653589793

ACONST=LATTICE CONSTANT (IN A.U.)
ALPHA=THE EXCHANGE PARAMETER
ELECT=NUMBER OF ELECTRONS PER ATOM

READ(5,10)ACONST,ALPHA,ELECT
10 FORMAT(6F12.8)

SC IDCUB=1, BCC IDCUB=2, FCC IDCUB=4
KZMAX=MAXIMUM MAGNITUDE OF \( (K \times ACONST/2/PI)^2 \)
NB, DIMENSION OF THE HAMILTONIAN AND OVERLAP ARE NB\*NB
KBDIV=DIVISION ALONG (1,0,0) DIRECTION IN THE B.Z.
IP (KBDIV, 1) POINTS BELONGING TO THE DOUBLE DIVISION ARE SORTED
TO APPEAR FIRST.
NKPRT=GE.NUMBER OF PERMUTED E.L.V. WITH K**2.LE.KZMAX.
NBUCB=NUMBER OF THE CORE STATES FOR EACH SPIN.
NBFBM=NUMBER OF BAND STATES FOR EACH SPIN.
NKPRN=NUMBER OF NFW DENSITY(K) CONSIDERED IN EACH ITERATION.
NKPICL=NUMBER OF CORRECTIONS TO V(K) INCLUDED WHEN CONSTRUCTING
THE NEW HAMILTONIAN.

===================================================================

IF (IETCTL.EQ.0) THE FUNCTION IS THE SAME AS THE FUNCTION OF SCF!
IETOTL=1 FOR THE VB POTENTIAL AND CALCULATION OF THE TOTAL
ENERGY
IETOTL=2 FOR \( \alpha/3 \) POTENTIAL AND CALCULATION OF THE TOTAL
ENERGY

===================================================================

READ(5,20)IDCUB,KZMAX,NB,KBDIV,KBBZPB,WKPRT
1,NBCB,J,MFBM,NKPRN,NKPICL,IETCTL
20 FORMAT(20I5)
OMEGA=ACONST**3/DFLOAT(IDCUB)
AK=-2.DO*PI/ACONST
AKF2=AK**2
AKFBZ=AKF/DFLOAT(KBDIV)
IF (IDCUB.EQ.1) AKFBZ=AKFBZ/2.DO
DSN=PHB&GA.LIOLA.SCF

METHOD=1.DO/3.DO

RINDEXB=NB*(NB+1)/2

R=\{\Omega=3.DO/(4.DO*PI)\}**G1NTHE

CODK1=-16.DO*PI*PI/(3.DO*OMEGA)

IF (IDCUB.NE.1) AHALF=ACONST/2.DO

IF (IDCUB.EQ.1) AHALF=ACONST

GENERATE EQUALLY SPACED FEINTS AND THE CORNER OF THE TETRAHEDRONS

IN 1/40TH OF THE INDEPENDENT BRILLIUSIN ZONE

IF (1.EQ.1)

CALL GB2PT(KX,KEY,KBZ,MT,NKBZPT,IDCUB,KL,SUN*,1,0,KBTWAR)

COEFF=OMEGA*(AMBDZ/PI)**3

COEF=COEFF/OMEGA

COEFF=1.DO/(OMEGA*SUN)

CALL TD2BPT(IPT,NKP,KL,IP2CL,KBX,KEY,KBZ,NOKEZPT,IDCUB)

NBTCL=NBCORE+ABERN

NBSI=NB-M with

NKT1=NST+ABERN-1

NCT1=NST1+1

NBNO=NBERN

CALL GPERM(KPERX,KPERY,KPERZ,KSDU,NKPTB,IDCUB,KMAXM,1,0)

READ IN THE NON-SELF-CONSISTENT FOURIER COEFFICIENTS OF THE

COULOMB., AND EXCHANGE POTENTIAL.

J=0

30 CONTINUE

J=J+1

READ(9) KS,GCoul,GEWAD,GEWAD,GEWAD,GEWAD,GEWAD,GEWAD,GEWAD,GEWAD

IGALU,IGFU,GDD,KSX(J),KSY(J),KSZ(J),KNB(J)

IF (IECTCL.EQ.1)

READ(9) KS,GCoul,GEWAD,GEWAD,GEWAD,GEWAD,GEWAD,GEWAD,GEWAD

GDD,IGDU,KSX(J),KSY(J),KSZ(J),KNB(J)

IF (KS.GT.4*KMAXM) GO TO 50

ALAMPA(J)=GAPA

ALAMUP(J)=GAPU

ALAMN(J)=GADN

ALAMJD(J)=GADU

ALAMDU(J)=GADD

IF (IECTCL.EQ.1) GO TO 35

DVALPA(J)=GAPA

DVPP(J)=GBPJ

DVLPD(N)=GADD

DVLPD(J)=GBDJ

DVLPDU(J)=GBDU

35 CONTINUE

II=KSX(J)+1

JJ=KSY(J)+1

KK=KSZ(J)+1

NK=NK+1

IF (J.GT.NKPTON) GO TO 30

KSDU(J)=KS
DSN=PHEAGA.LIOLA.SCF

```plaintext
DKUP0(J)=GDD
DKDON(J)=GDD
IF(KS.EQ.0) GO TO 40
AA=AARF*DFLOAT(KS)
AA=8.0D0*PI/AA
VKNO(J)=GEXDN
VKUPO(J)=GEXUP
IF (IETOTL.EQ.1) WUPO(J)=GWUP
IF (IETOTL.EQ.1) WDNO(J)=GWDN
VKO(J)=GCODL+AA*ELECT/CHEGA
GO TO 30
40 WUPO(J)=GEXUP
WDO(J)=GEXDN
IF (IETOTL.EQ.1) WUPO(J)=GWUP
IF (IETOTL.EQ.1) WDNO(J)=GWDN
VKO(J)=GCODL
GO TO 30
50 NKPT=J-1
WRITE(6,60) ACCEPT,ALPHA,ELECT,WKPT,WKPTP,IKDGB,KBZDIV,
NKBZAF,NS,ITPOL,WKPI
60 FORMAT (IX,'LATTICE CONST=',F10.5,2X,'EXCH PARA=',F10.5,2X,
'ELECT NO=',FK,2.2X,'WKPT=',I5,2X,'K STAR=',I5,2X,'K NO=',I5,2X,
'KZAF=',I5,2X,'3D NO=',I5,2X,'INCLUDED K=',I5,2X)
DO 70 J=1,NKPT
70 JI=IABS(JI)
JK=IABS(JK)
KK=IABS(KK)
REWIND 8
IF (IETOTL.EQ.1) REWIND 9
DO 80 IRLV=1,KBZPT
DKUPCD(IRLV)=0.0D0
DKDOND(IRLV)=0.0D0
CVKOD(IRLV)=0.0D0
CXPDCD(IRLV)=0.0D0
CXXMOD(IRLV)=0.0D0
80 CONTINUE
```

C FACTO0, FACTO, and FACT are parameters used to modify the potential
C in order to speed up the iterative procedure.
C FACTO is the FACTO used in iteration ITEROD.
C FACTO modifies the potential obtained in iteration ITEROD before
C constructing the new Hamiltonian for iteration ITEROD+1.
C FACT modifies the new potential obtained in iterations ITEROD+1 to
C ITERM.
C PERFORM ITERATION NUMBER ITERCD+1 IN ITERAW.
C IF (NPART.EQ.0) PERFORM THE COMPLETE CALCULATION.
C IF (NPART.GT.0) ENERGY BAND HAS ALREADY BEEN CALCULATED
C IF (NPART.EQ.1) CALCULATE DENSITY(K) and EXCH(K)
C IF (NPART.EQ.2) CALCULATE EXCH(K) ONLY.
C IF (NPART.EQ.3) CALCULATE DENSITY(K) ONLY.
C IF (NPART.LE.0 AND NKBZST.EQ.0) B.Z. POINTS NKBZST AND NKBZED ARE
C DETERMINED AUTOMATICALLY.

```

---

FACTO0 IS THE FACTO USED IN ITERATION ITEROD.
FACTO MODIFIES THE POTENTIAL OBTAINED IN ITERATION ITEROD BEFORE
CONSTRUCTING THE NEW HAMILTONIAN FOR ITERATION ITEROD+1.
FACT MODIFIES THE NEW POTENTIAL OBTAINED IN ITERATIONS ITEROD+1 TO
ITERM.
PERFORM ITERATION NUMBER ITERCD+1 IN ITERAW.
IF (NPART.EQ.0) PERFORM THE COMPLETE CALCULATION.
IF (NPART.GT.0) ENERGY BAND HAS ALREADY BEEN CALCULATED
IF (NPART.EQ.1) CALCULATE DENSITY(K) AND EXCH(K)
IF (NPART.EQ.2) CALCULATE EXCH(K) ONLY.
IF (NPART.EQ.3) CALCULATE DENSITY(K) ONLY.
IF (NPART.LE.0 AND NKBZST.EQ.0) B.Z. POINTS NKBZST AND NKBZED ARE
DETERMINED AUTOMATICALLY.

---

Addressing the code, the provided snippet represents an input file for performing a computational procedure, likely related to electronic structure calculations, as per the context of the DSN. It contains sections defining variables, initializing arrays, and implementing conditional logic for different scenarios, such as initial calculations, energy band calculations, density calculations, and exchange calculations. The code also hints at the potential use of factoring to accelerate iterations, as indicated by the presence of parameters FACTO0, FACTO, and FACT, which are used to modify the potential. The comments guide through the decision-making process, ensuring that the calculations proceed according to specific conditions and parameters, which is a common practice in computational science to optimize performance and accuracy.
IF (NPABT.EQ.-1) CALCULATE BANDS FROM NKBZST TO NKBZED ONLY.
IF (NPABT.EQ.-2) CALCULATE BANDS FROM NKBZST TO NKBZED AND DENSITY.
IF (NPABT.EQ.-3) CALCULATE BANDS FROM NKBZST TO NKBZED, DENSITY, AND EACH(R).
IF (NPABT.EQ.-4) CALCULATE BANDS AT NKBZST+1 AND NKBZED ONLY.
IF (IPUN.NE.0) PUNCH THE CHARGE DENSITY AND THEIR FOURIER COEFFICIENTS.
IF (IETFNL.NE.0) ENERGIES AND WAVE FUNCTIONS OF ALL NB STATES ARE
SAVED IN OUTPUT CHANNEL FILEPO01 (IN SINGLE PRECISION).

90 READ (5,100,END=780) FACTO,FACTO,FACTO,ITEROD,ITEROD,MPART,
  NKBZST,NKBZED,IPUN,IBDFNL
100 FORMAT (5F10.5,1015)
110 CONTINUE
  IF (NPABT.EQ.0) GC TO 160
  IF (NPABT.IE.0) GO TO 130
C TEST THE NUMBER OF B.Z. POINTS AT WHICH ENERGIES AND WAVE
FUNCTIONS HAVE BEEN CALCULATED.
  DO 120 NM=1,NKBZST
  DO 120 II=1,NBTOI
    READ (2) ENGU,(XUP(JJ,II),JJ=1,NB)
    ENGD,(XDN(JJ,II),JJ=1,NB)
    IF (II.GT.NDYNED) GO TO 120
    ENG(JJ,II)=ENGU
    EDN(JJ,II)=ENGD
120 CONTINUE
  rewind 2
  GO TO 170
130 IF (NKBZST.NE.0) GO TO 170
  DO 140 NM=1,NKBZPT
  NKBZST=NM
  DO 140 II=1,NBTOI
    READ (2,END=150) ENG,(XUP(JJ,II),JJ=1,NB),ENGD,(XDN(JJ,II),JJ=1,NB)
140 CONTINUE
  rewind 2
  NPART=1
  GO TO 110
150 CONTINUE
  rewind 2
  NKBZED=NKBZPT
  GO TO 170
160 CONTINUE
  NKBZST=1
  NKBZED=NKBZPT
170 CONTINUE
  IF (ITEROD.EQ.0) GO TO 240
C READ THE CORRECTIONS DUE TO SELF-CONSISTENCY IN THE PREVIOUS
C ITERATION AND MODIFY THEM WITH FACTO BEFORE CONSTRUCTING THE
C NEW POTENTIAL.
  DO 220 I=1,ITEROD
    READ (19,END=250) (DCOKUP(J),DVAKUP(J),CCCKDN(J),DVAKDN(J),J=1,
    NKBZPT)
    READ (19,END=260) (CDKUP(J),CDKN(J),CVDN(J),CDVK(J),DKDNN(J),
    J=1,NKFIN)
    IF (I.NE.ITEROD-2) GO TO 190
DSN=PHBAGA_DIOIA.SCF

DO 180 J=1,NKPT
CVKOD(J)=CVKNN(J)
CKUPOD(J)=CKUPNW(J)
CKDNOD(J)=CKDNNW(J)
DKUPOD(J)=DKUPNW(J)
DKDNOD(J)=DKDNNW(J)
180 CONTINUE
190 CONTINUE
IF (IKEQ=0) GO TO 210
DO 200 KN=1,NKPT
DKUPOD(KN)=FACT0*DKUPNW(KN)+(1.D0-FACT0)*DKUPOD(KN)
DKDNOD(KN)=FACT0*DKDNNW(KN)+(1.D0-FACT0)*DKDNOD(KN)
CVKOD(KN)=FACT0*CVKNN(KN)+(1.D0-FACT0)*CVKOD(KN)
CKUPOD(KN)=FACT0*CKUPNW(KN)+(1.D0-FACT0)*CKUPOD(KN)
CKDNOD(KN)=FACT0*CKDNNW(KN)+(1.D0-FACT0)*CKDNOD(KN)
200 CONTINUE
210 CONTINUE
DO 230 KN=1,NKPT
DKUPOD(KN)=FACT0*DKUPNW(KN)+(1.D0-FACT0)*DKUPOD(KN)
DKDNOD(KN)=FACT0*DKDNNW(KN)+(1.D0-FACT0)*DKDNOD(KN)
CVKOD(KN)=FACT0*CVKNN(KN)+(1.D0-FACT0)*CVKOD(KN)
CKUPOD(KN)=FACT0*CKUPNW(KN)+(1.D0-FACT0)*CKUPOD(KN)
CKDNOD(KN)=FACT0*CKDNNW(KN)+(1.D0-FACT0)*CKDNOD(KN)
230 CONTINUE
240 CONTINUE
GO TO 270
250 ITEROD=1-I
NPAR=0
FACT0=1.D0
FACT00=1.D0
GO TO 160
260 ITEROD=1
NPAR=2
FACT0=1.D0
FACT00=1.D0
GO TO 110
270 ITERST=ITEROD+1
WRITE(6,280) ITERST,FACT00,FACT0,NPAR
280 FORMAT(1H1,14,'ITERST=',13,5X,'FACTO0=',P6.3,5X,'FACT0=',P6.3,
            8X,'NPAR=',15,I5,'//')
DO 770 ITERST=ITERST+1
IF (NPAR.GT.0.AND.ITERST.EQ.ITEREST) GO TO 490
290 CONTINUE
DO 460 NM=1,NKZ
WRITE(6,300) KEX(NM),KEY(NM),KBZ(NM),NM
300 FORMAT(1H3,N3,3I16,5X,5X,5X,15,I5,'//')
IF (NM.EQ.0.AND.NM.EQ.NKZ+1.AND.NM.EQ.NKZED) GO TO 410
IF (NM.EQ.-4.AND.NM.EQ.-NKZ+1.AND.NM.EQ.-NKZED) GO TO 410
310 FORMAT(64A)

C READ THE ORIGINAL COULCHEM, KINETIC, EXCHANGE, AND OVERLAP MATRICES
C
DO 320 IJ=1,NBTRI
READ(4,310) GC,GX,GU,GD,GK,G0
HUP(IJ)=GC*GK+GU*ALPHA
HDN(IJ)=GC*GK+GD*ALPHA
OV(IJ)=G0
DSN=PBAGA.LIOLA.SCF

320 CONTINUE 
   IF (ITFL.EQ.1) GO TO 350
C
   CALCULATE THE HAMILTONIAN RETAINED FROM LAST ITERATION BY THE 
   GENERALIZED OVERLAP MATRICES.
C
   DO 340 IRLV=1,KKFRNM
         READ (I) KS,KT,SJJ
         IF (IRLV.GT.NKPLIC) GO TO 340
         AA=CYKOD(IRLV)*CXUPCD(1PLV)*ALPHA
         BB=CYKOD(IRLV)*CXDNOD(IRLV)*ALPHA
         DO 330 IJ=1,NBTBI
            HUP(IJ)=HUP(IJ)+AA*SIJ(IJ)
            HDN(IJ)=HDN(IJ)+BB*SIJ(IJ)
         CONTINUE
330 CONTINUE
   DO 340 CONTINUE
340 CONTINUE
   IF (ITFL.EQ.1) GO TO 350
C
   DO 360 II=1,NBST,NB 
         WRITE (2) HUP(II),(XUP(JJ,II),JJ=1,NE) 
         WRITE (2) HDN(II),(XDN(JJ,II),JJ=1,NE) 
         I=II-KBST*1
         IF (I.CT.KBST.F07) GO TO 360
         EUP(I,NIt)=EUP(II)
         EDN(I,KI)=EDN(II)
   CONTINUE
360 CONTINUE
   IF (IIBFLN.EQ.0) GO TO 460
   DO 380 II=1,NB 
         GUP=HUP(II)
         DO 370 JJ=1,NB 
            GUP(JJ)=XUP(JJ,II)
            WRITE (10) GUP,EDU,EDN 
         CONTINUE 
370 CONTINUE
   DO 390 JJ=1,NB 
         GDN=HDN(II)
         GDN(JJ)=XDN(JJ,II)
         WRITE (10) GDN,EDU,EDN 
   CONTINUE 
390 CONTINUE
   WRITE (10) GDN,EDU,EDN 
         GO TO 460 
410 DO 420 JJ=1,NBTBI 
420 READ (4,310) GCG,GX,GU,GD,GK,GO
   CONTINUE
430 CONTINUE
   IF (IIBFLN.EQ.0) GO TO 460
   DO 440 I=1,NBTOL 
         READ (2) ENGU,(XUP(JJ,1),JJ=1,NE),ENGU,(XDN(JJ,1),JJ=1,NE)
         IF (II.GT.NSBFRNM) GO TO 440
         EUP(II,NM)=ENGU
         EDN(II,NM)=ENGU 
   CONTINUE
440 CONTINUE
   IF (IIBFLN.EQ.0) GO TO 460
   DO 450 KSB=1,2
DO 450 II=1,NB
450 READ(10,END=470) GEDP,GXUP
460 CONTINUE
   GO TO 480
470 NKEZST=NM
   REWIND 1
   REWIND 2
   REWIND 10
   GO TO 290
480 IF (NPART.EQ.-1 OR NPART.EQ.-4) STOP
   REWIND 1
   REWIND 2
   REWIND 10
C
C DETERMINE THE FERMI ENERGY
C
490 IF (NFERM.EQ.0) GO TO 500
   NSPIN=2
   NKB=ELECT-2*NCORE
   CALL FERMI(E,EDN,NFERM,NKEZET,IP1,IPR1,NP1,ELC,NSPIN,FERMI)
500 CONTINUE
   IF (NPRINT.EQ.1 .AND. ITER.EQ.ITERST) GO TO 650
C
C CALCULATE FOURIER TRANSFORM OF CHARGE DENSITY
C THE B.Z. INTEGRATION FOR THE CORE STATES ARE OBTAINED BY HISTOGRAM
C METHOD AND THE FINE STATES BY ANALYTICAL TETRAHEDRON METHOD.
C
DO 510 IRLV=1,NKPTRN
   DCOKUP(IRLV)=0. DO
   DCOKDN(IRLV)=0. DO
510 CONTINUE
   DO 570 IN=1,NKZPT
      READ(2) INGU,(XUP(JJ,II),JJ=1,NB)
   6 DO 520 IY=1,NKZPT
      READ(2) INGU,(XUP(JJ,II),JJ=1,NB)
520 CONTINUE
   DO 570 IRLV=1,NKPTRN
      READ(1) K5,KT,SIJ
      DO 560 IJ=1,NBTOIL
   8 AA=0. DO
      BB=0. DO
   9 LJ=0
      DU 540 IJ=1,NB
      DO 540 IJ=1,11
         LJ=IJ+1
         AC=XUP(IJ,IN)*SIJ(IJ)*XUP(II,IN)
         BC=XDN(IJ,IN)*SIJ(IJ)*XDN(II,IN)
      IF (IJ.EQ.12) GO TO 530
         AC=AC*2.D0
         BC=BC*2.D0
   530 AA=AA*AC
      BB=BB+BC
540 CONTINUE
   IF (IN.LT.NBFERM) GO TO 550
   DCOKUP(IRLV)=DCOKUP(IRLV)+AA*WT(NM)
   DCOKDN(IRLV)=DCOKDN(IRLV)+BB*WT(NM)
DSN=PHBAGA,DIOLA,SCF

GO TO 560
550 IF(IPUR.NE.0) STOP
DO 560 KPART=1,NKPT
550 CONTINUE
560 CONTINUE
WRITE(6,580)
580 FORMAT((1X,'X2,2X,'COND*,2X,'KEY*,2X,'KB1*,2X,'KB2*',2X,'KPT*,2X,'3X,'DENSITY UP',2X,'NEW DENSITY UP',2X,'COND*,2X,'KEY*,2X,'KB1*,2X,'KB2*'),/)
SDUP=0.DO
SDDN=0.DO
DO 630 IRLV=1,NKPT
AA=1.DO/KNB(IRLV)
IF(NENO.EQ.0) GO TO 600
DO 590 NK=1,NENO
DO 590 KPI=1,NKBP
YDN(NK,KPT)=EHDN(IRLV,NK,KPT)
590 CONTINUE
WRITE(6,610) IRLV,KSX(IRLV),KSY(IRLV),KSZ(IRLV),DKUPO(IRLV),SUP,
& SUMUP,CUMUP,CUMDN,SUP,CUMUP,CUMDN
IF(IPUR.NE.0) STOP
WRITE(6,620) IRLV,KSX(IRLV),KSY(IRLV),KSZ(IRLV),SUMUP,CUMUP,
& SUMDN,CUMDN
610 FORMAT((15,8F13.6))
620 FORMAT((15,4E15.8))
630 CONTINUE
WRITE(19) (DCOKUP(J),DVAKUP(J),DCOKDN(J),DVAKDN(J),J=1,NKPT)
AELC=(DCOKUP(1)+DVAKUP(1)+DCOKDN(1)+DVAKDN(1)) *OMEGA
AMAG=(DCOKUP(1)+DVAKUP(1)-DCOKDN(1)-DVAKDN(1)) *OMEGA
WRITE(6,640) AELC,AMAG
640 FORMAT(/,1X,'ELECT*',1X,'MAGNETH. MO*',1X,'F10.6,5X,'F10.6) GO TO 660
650 CONTINUE
WRITE(19) (DCOKUP(J),DVAKUP(J),DCOKDN(J),DVAKDN(J),J=1,NKPT)
660 CONTINUE
IF(NPART.EQ.-2.OR.NPART.EQ.3) STOP
BACKEND 1

C
C MODIFIED THE SELF-CONSISTENT CORRECTIONS TO IMPROVE CONVERGENCE.
C
DO 670 KN=1,NKPT
DKUPNW(KN)=DKUPW(KN)+DVAKUP(KN)-DKUPO(KN)
DSN = PHAGA.LIOLA.SCF

\[\begin{align*}
D_{KDNW}(KN) &= D_{KDN}(KN) + D_{SKDN}(KN) - D_{DKDO}(KN) \\
D_{KUPW}(KN) &= \text{FACT} \times D_{KUPN}(KN) + (1.00 - \text{FACT}) \times D_{KUPD}(KN) \\
D_{KDNW}(KN) &= \text{FACT} \times D_{KDNW}(KN) + (1.00 - \text{FACT}) \times D_{KDNW}(KN)
\end{align*}\]

670 CONTINUE

CALCULATE THE CORRECTION TO THE EXCHANGE POTENTIAL.

DO 690 KN = 1, NNPRT
    SUMUP = 0.00
    SUMDN = 0.00
    SUMUP = 0.00
    SUMDN = 0.00
    DO 680 J = 1, NNPRT
        II = KSX(KN) - KPS(XJ(J))
        JJ = KSY(KN) - KPS(YJ(J))
        KK = KSZ(KN) - KPS(ZJ(J))
        JJ = 1ABS(JJ) + 1
        J = 1ABS(JJ) + 1
        K = 1ABS(KK) + 1
        KS = NKP(II, JJ, KK)
        KT = KS1GP(JJ)
        SUBUP = SUMUP + ALAMUP(KS) \times D_{KUPN}(KT) + ALAMDC(KS) \times D_{KDNW}(KT) \\
        SUMDN = SUMDN + ALAMDN(KS) \times D_{KDNW}(KT) + ALAMDU(KS) \times D_{KUPN}(KT)
    IF (IETOTL.EQ.1) SUMUP = SUMUP + D_KUPUP(KS) \times D_{KUPD}(KT) * D_{KUPN}(KT) \\
    IF (IETOTL.EQ.1) SUMDN = SUMDN + D_KDNUP(KS) \times D_{KDNP}(KT) * D_{KUPN}(KT)

680 CONTINUE

C XUPN(KN) = SUMUP
C XDNW(KN) = SUMDN

690 CONTINUE

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

AA = 0.00
RO = R0 * RO
R0 = RG * RC
DO 700 J = 2, NNPRT
    KK = AK2 + KSD(U(J))
    RK = DSQR(RK2)
    RK3 = RK1 + RK2
    RK4 = RK2 + RK2
    RO = RG * RK
    CO = (D_KUPN(J) + D_KDNW(J)) \times KNB(J)
    AA = AA + CO * RK1 \times \{(3.00-RO2/RK2-6.00/RK4) \times \text{DSIN}(RK) + \\
    6.00 * RG/RK3-F/3/RK2) \times \text{ECCS}(RK)\}

700 CONTINUE

C VRNW(J) = CODK1 * AA

PRINT FOURIER COEFFICIENTS OF THE NEW POTENTIAL.

710 FORMAT (1X, 'ITERATION=', I3, 5X, 'FACTO=', F6.3, 5X, 'FACT=', F6.3, 5X, 
    'NFAM=', I5, 5X, 'I15', 5X, I3, 5X)
WRITE (6, 710) ITER, FACTO, FACT, NPART
WRITE (6, 720)

do 725 k=1,ns
    anucle=0.0
    do 740 j=1,nkp
      if (k.eq.1) go to 730
      bk2=akr2*ksq(j)
      anucle=-k*elect/omega
      continue
      write(6,750) kss(j),ksy(j),ksz(j),anucle,vko(j),cvknn(j),cvkod(j)
      write(6,735) kss(j),ksy(j),ksz(j),cvknn(j),cvkod(j)
      continue
      write(11,12,211,4) (1x,f9.6)
      continue
      if (ipun.ne.0) go to 810
      continue
      write(11,12,211,12) (1x,f9.6)
      continue
      do 800 j=1,nkp
        write(17) (ks2(j),knb(j),vko(j),cvknn(j),j=1,nkp)
        continue
        write(37) (vxdn(j),cxdnw(j),ckdnw(j),j=1,nkp)
APPENDIX A.3: New Version of PROGRAM DENST

DSN=PHBAGA.LIOILA.DEN

//PHBAGA54 JOB 1103,60245,004,2)*PH.DIGIAN,MSGCLASS=S,
//NOTIFY=PHBAGA
//AFTER FEFB254
//ROUTE PRINT PHYSICS
//JOBPARM SHIFT=D
//EXEC FORTHCLG,PARM.POLT='NOSOURCE,LANGIVL(66),OPT(2)',
//PARM.LKED='NO',REGION=1200K,TIME=999
//FORT.SYSIN DD *

PROGRAM DENST
THE SIXTH PART OF
A GENERAL PROGRAM TO CALCULATE SELF-CONSISTENT ENERGY BANDS
USING THE MODIFIED TIGHT BINDING OR ICQC METHOD
BY
C.S. WANG AND J. CALLAWAY
TOTAL ENERGY CALCULATION
BY
J. CALLAWAY, X. ZOU, AND D. BAGAYOKO
DEPARTMENT OF PHYSICS
LOUISIANA STATE UNIVERSITY
BATON ROUGE LOUISIANA 70803

ROUTINES USED IN DENST
FERMIE (FROM PROGRAM SCF1)
GZ2PT (FROM PROGRAM FCOF)
TDZ2PT (FROM PROGRAM SCF1)
TDENS (FROM PROGRAM SCF1)
TDVL (FROM PROGRAM SCF1)
TELECT (FROM PROGRAM FCOF)

INPUT/OUTPUT CHANNELS USED IN DENST
PT01F001 ENERGIES AND WAVE FUNCTIONS.
(OUTPUT CHANNEL PT02F001 OF PROGRAM BND OR
OUTPUT CHANNEL TT10F001 OF PROGRAM SCF1 OR SCF2)
PT05F001 CARD READER.
PT06F001 LINE PRINTER.

CALCULATE THE DENSITY OF STATES BY THE LINEAR ANALYTICAL
TETRAHEDRON METHOD.
**DSN=PHBAGA.DICLA.DEN**

---

**DIMENSION RESTRICTIONS.**

1) IPT(I), IPTO L WHERE IPTCL IS THE NUMBER OF TETRAHEDRONS IN 1/4TH OF THE B.Z.

2) NKBZPT, DIMENSION OF KBX, KBY, KBZ

3) NP(I,J,I), I = KBZDIV + 1

4) FUP(NDFERM, N3), EUPL(NDFERM, NKBZPT), GX(N3)

5) NMAX, DIMENSION OF EN, SWUP, SWDN, TUDP, TDND.

---

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

**INTEGER*2 KX1, KY1, KZ1, KNE**

**INTEGER*2 IPT(4,2008), KBX(506), KBY(506), KBZ(506), NP(21,21,21)**

**REAL*4 SIJ(0346)**

**DIMENSION EUPL(15,506), EDK(15,506), GX(43), GX1(43)**

**DIMENSION EN(1801), SWUP(1801), SWDN(1801), TUDP(1801), TDND(1801)**

**ELSEU(1801), ELSE(1801), SW(1801)**

**DIMENSION CVK(40), DWUP(40), DUDP(40), DUNCUP(40), VXCP(40), VXCDN(40)**

**DIMENSION EN(1801), SVUP(1801), SWDN(1801), TUDP(1301), TDND(1801)**

**ELSEU(1801), ELSEN(1801), SH(1801)**

**DIMENSION CVKNW(40), DHDP(40), DPDN(40), VCXD(40), VXCDN(40), EVDN(40)**

---

**NMAX=NUMBER OF DIVISION IN ENERGY AT WHICH THE DENSITY OF STATES ARE CALCULATED.**

**KBZDIV=DIVISION ALONG (1,0,0) DIRECTION IN THE B.Z.**

**KBZHAF=NUMBER OF POINTS BELONGING TO THE DOUBLE DIVISION ARE SORTED TO APPEAR FIRST.**

**SC IDCUB=1, ECC IDCUB=2, FCC IDCUB=4**

**NSPIN =1 AND 2 FOR PARAMAGNET AND FERROMAGNET RESPECTIVELY.**

**NDFERM=NUMBER OF BAND STATES FOR EACH SPIN.**

**NB=NUMBER OF THE CORE STATES FOR EACH SPIN.**

**NKBXDIMENSION OF THE HAMILTONIAN AND OVERLAP ARE NB**

**IF(IDISC.NE.0) ENERGIES ARE READ FROM CHANNEL.Trim0103.**

**IF(IDISC.EQ.0) ENERGIES ARE READ FROM CARDS.**

---

**IF(IETOTL.EQ.1) CALCULATE THE TOTAL ENERGY AND USE VHF POTENTIAL**

**IF(IETOTL.EQ.2) CALCULATE THE TOTAL ENERGY AND USE ALPHA=2/3 POT.**

**IF(IETOTL.EQ.0) THE FUNCTION IS THE SAME AS THE FUNCTION OF DENS**

**IF(NDENS.EQ.0) THE DENSITY OF STATES IS NOT CALCULATED**

---

**READ(5,333) NDENS, IETOTL**

**FORMAT(1015)**

**READ(5,10) NMAX, KBZDIV, KBZHAF, IDCUB, NSPIN, NDFERM, NBcoe, NE, IDISC**

**FORMAT(1015)**

---

**EMIN=MINIMUM ENERGY CONSIDERED.**

**DE=STEPS IN THE ENERGY DIVISION.**

**ZDEC=ENERGY DIFFERENCE IS LESS THAN ZERO THAN ENERGIES ARE CONSIDERED EQUAL.**

**ELECT=NUMBER OF BAND ELECTRONS PER ATOM**

**READ(5,20) EMIN, DE, ZDEC, ELICT, Z, ACOST**
DSN=PhBAGA.DIOL.DEN

---

C

AAA=ACONST**3
OMEGA=AAA/DFLOAT(IDCUB)
FO=Z/OMEGA
WBN2=WFERM
WBTOL=NEFERS+WFERM
NBST=NB-WBTOL+1
ENDT=NBST+WFERM-1
NBTI=NB*(NB+1)/2

20 FORMAT (10F10.5)
COAST=E. DO/DPLCAT(IDCUB*KBZDIV**3)
IF (IDCUB.EQ.1 ) CONST=CONST/6. DO
IF (NSPIN.EQ.1 ) CONST=CONST*2. DO
CON=CONST*3. DO
PI=3.141592653589793
K=KBZDIV+1
CALL GEZPT(KBX,KEY,KBZ,WT,NKBZPT,IDCUB,KSUN,0,0,KZHAF)
IF (IDISC.ME.0 ) GO TO 50
DO 30 K=1,NKBZPT

EUP=BAND STATES ENERGIES OF MAJORITY SPIN.
KX= X COMPONENTS OF K POINTS IN THE E.Z.
KY= Y COMPONENTS OF K POINTS IN THE E.Z.
KZ= Z COMPONENTS OF K POINTS IN THE E.Z.

READ (5,40 ) (EUP(I,K),I=1,NEFERM),KX,KY,KZ
KBX(K)=KX
KBZ(K)=KY
NKBZPT=KZ
IF (NSPIN.EQ.1 ) GO TO 30

EDN=BAND STATES ENERGIES OF MINORITY SPIN.

READ (5,40 ) (EDN(I,K),I=1,WFERM)

GO TO 80

CONTINUE

50 CONTINUE
DO 70 K=1,NKBZPT
DO 60 J=1,NISP
READ (1) GEENG,GX
IF (J.LT.NBST.OB.J.GT.NBEND) GO TO 60
IF (NSPIN.EQ.1 ) EUP(J-NBST+1,K)=GENG
IF (NSPIN.EQ.2 ) EDN(J-NBST+1,K)=GENG

60 CONTINUE

70 CONTINUE
RENEW 1

80 CONTINUE

WRITE(6,810) IDCUB,KBZDIV,NEMAX,EMIN,DE,IPCL,NEFERS,WEFERS,WE

810 FORMAT (1X,ATOM/CUBE='15,3X,'B.Z.DIV='15,3X,'ME='15,3X,'M='15,3X,
2*EMIN='15,3X,'DE='15,3X,'TD NC='15,3X,
2*B.Z.PT='15,3X,'CORE='15,2X,'EMAD='15,2X,'MB='15,2X)
DSN=FPeBAGA: DIOLA.DEN

CALL FERMIE(PUP,EDA,NBFEEM,NKZPT,IP,IPCL,CONST,ELECT,NSPIN,ETERN)

C CALCULATE THE AVERAGE SINGLE ELECTRON ENERGY, D, O AND THE
C EXCHANGE-CORRELATION ENERGY

C IF (IP = 0) GO TO 99

C READ IN K2*1/A/2PI AND THE NON-SELF-CONSISTENT FOURIER
C COEFFICIENTS OF THE COULOMB AND EXCHANGE POTENTIALS.

C IF (NSPIN.EQ.2) GO TO 814

READ (17) (K2(J),KNE(J),VKO(J),CVKN(J),J=1,NKPTRN)
READ (17) (VXCUP(J),DVXCUP(J),DPUP(J),J=1,NKPTRN)
READ (27) (K2(J),KNB(J),VKO(J),FPUP(J),J=1,NKPTRN)
READ (27) (WUP(J),DWUP(J),DPUP(J),J=1,NKPTRN)

814 CONTINUE

IF (NSPIN.EQ.1) GO TO 818

READ (27) (K2(J),KNB(J),WDN(J),DWN(J),J=1,NKPTRN)
READ (27) (UP(J),D UP(J),FPUP(J),J=1,NKPTRN)
READ (37) (K2(J),KKB(J),PDNO(J),DEFN(J),J=1,NKPTRN)
READ (37) (VXCNO(J),DVXCDN(J),DPDN(J),J=1,NKPTRN)

818 CONTINUE

WRITE (6,820)

820 FORMAT (/,'K(J) = K(J) + K(J)')
WRITE (6,824)

824 FORMAT ('KNB(J) = KNB(J) + KNB(J)')
WRITE (6,828)

828 FORMAT (/,'VKO(J) = VKO(J) + VKO(J)')
WRITE (6,858) (VKO(J),J=1,NKPTRN)

VCKO(1)=VKO(1)
DO 830 J=2,NKPTRN
  K(J+1)=K(J)+30.8J
AKS2=(2.0D0*PI/ACONST)**2*DPLOAT(AK)
  VCKO(J)=VKO(J)-AKS2
830 CONTINUE

WRITE (6,834)

834 FORMAT (/,'CVKN(J) = CVKN(J) + CVKN(J)')
WRITE (6,858) (CVKN(J),J=1,NKPTRN)
WRITE (6,838)

838 FORMAT (/,'VXCO(J) = VXCO(J) + VXCO(J)')
WRITE (6,858) (VXCO(J),J=1,NKPTRN)
WRITE (6,840)

840 FORMAT (/,'DVXC(J) = DVXC(J) + DVXC(J)')
WRITE (6,858) (DVXC(J),J=1,NKPTRN)
WRITE (6,844)

844 FORMAT (/,'VKO(J) = VKO(J) + VKO(J)')
WRITE (6,858) (VKO(J),J=1,NKPTRN)
WRITE (6,848)

848 FORMAT (/,'DV(J) = DV(J) + DV(J)')
WRITE (6,858) (DV(J),J=1,NKPTRN)
WRITE (6,850)

850 FORMAT (/,'DENS(J) = DENS(J) + DENS(J)')
WRITE (6,858) (DENS(J),J=1,NKPTRN)
WRITE (6,854)

854 FORMAT (/,'DP(J) = DP(J) + DP(J)')
WRITE (6,858) (DP(J),J=1,NKPTRN)
WRITE(6,858) (DPUP(J),J=1,NKPTRN)
858 FORMAT(1X,10P3.6)
   IF(NSPIN.EQ.1) GO TO 884
   WRITE(6,860)
860 FORMAT(1X,'VXCDN(J), J=1,NKPTRN')
   WRITE(6,858) (VXCDN(J),J=1,NKPTRN)
   WRITE(6,864)
864 FORMAT(1X,'VXCDN(J), J=1,NKPTRN')
   WRITE(6,858) (VXCDN(J),J=1,NKPTRN)
   WRITE(6,870)
870 FORMAT(1X,'VXCDN(J), J=1,NKPTRN')
   WRITE(6,858) (VXCDN(J),J=1,NKPTRN)
   WRITE(6,874)
874 FORMAT(1X,'VXCDN(J), J=1,NKPTRN')
   WRITE(6,858) (VXCDN(J),J=1,NKPTRN)
   WRITE(6,878)
878 FORMAT(1X,'VXCDN(J), J=1,NKPTRN')
   WRITE(6,858) (VXCDN(J),J=1,NKPTRN)
   WRITE(6,882)
882 CONTINUE
C   IF(NSPIN.EQ.2) GO TO 888
C   IF(IETOTL.WE.2) GO TO 89
C   DO 89 J=1,NKPTRN
C      UP(J)=UP0(J)*2.DO/3.DO
C      DPUP(J)=DPUP0(J)*2.DO/3.DO
C   DRUP(J)=DRUP0(J)*2.DO/3.DO
C   89 CONTINUE
C   IF(IETOTL.WE.2) IFXCH=IFXCH/4.DO ??
888 CONTINUE
C
C CALCULATE THE AVERAGE SINGLE ELECTRON ELECTRON ENERGY
C
   CALL SUMOVK(EUP,IPT,IPTOL,KDX,KDY,KBZ,EDF,NKBDPT,ESNLG0,CCONST,
      EFERMI,NBNO)
   IF(NSPIN.EQ.1) GO TO 890
   CALL SUMOVK(EDM,IZ,IITCL,KEZ,KEZ,EDM,NKBDPI,ESNLG0,CCONST,
      EFERMI,NBNO)
   ESNLG0=ESNLG0+ESNLG0
   IF=UPD0(1)+PDNO(0.1)+DPUP(1)+DPDN(1)
890 CONTINUE
C   WRITE(6,894) NBKBDPT,NKBDT,ND,IETOT1,ACONST,FERMI,ESNLG0,
      IF,OMEGA
894 FORMAT(1X,'NO. KS=1,I3,2X,'NO. KS=1,I3,2X,'ND=1,I3,2X,'LATTICE. CONST.=1,F7.4,2X,
   *FERMI=1,F9.6,2X,*SINGLE. ELL. 1=1,F13.7,2X,
   *DENS OF KO=1,F9.7,2X,*CELL V=1,F8.4,')
C
C CALCULATE DU AND EXCHANGE-CORRELATION ENERGY AND THE CORRECTIONS
C BY CONSIDERING MORE KS POINTS. AND CALCULATE THE TOTAL ENERGY.
C
WP1=0.DO
WP2=0.DO
WCP1=0.DO
WCPD1=0.DO
WP1=0.DO
&DPUP1=0.DO
DSM=PHBAGA.DIOLA.DEN

WPDN=0. DO
VCESUM=0. DO
VPSUM=0. DO
VCPDSM=0. DO
VCPD=0. DO
WP SUM=0. DO
WPSUM=0. DO
VCPD=0. DO
VCPD=0. DO
VCPD=0. DO
NPT=0
898 CONTINUE
IF (NSPIN.EQ.1) GO TO 900
READ (11, END=934) KSC, GCOLT, GEWLD, GECH, GEXUP, GEXDN, GDSFA, GDSUP,
& GDSUP, GDSUP, GDSUP, GDSUP, GDSUP, GDSUP
& NPT=0
WRITE (6, 904) KSC, GCOLT, GEWLD, GECH, GEXDF, GEXDF, GEXDN, GDSFA, GDSUP,
& GDSUP, GDSUP, GDSUP, GDSUP, GDSUP, GDSUP
& NPT=0
IF (IEICTL.EQ.1) GO TO 900
READ (12, END=934) KSC, GCOLT, GEWLD, GECH, GEXUP, GEXDN, GDSFA, GDSUP,
& GDSUP, GDSUP, GDSUP, GDSUP, GDSUP, GDSUP
& NPT=0
WRITE (6, 905) KSC, GCOLT, GEWLD, GECH, GEXDF, GEXDF, GEXDN, GDSFA, GDSUP,
& GDSUP, GDSUP, GDSUP, GDSUP, GDSUP, GDSUP
& NPT=0
C
908 CONTINUE
C
IF (IEICTL.EQ.2) GECH=GECH*2. DO/3. DO
NWB=1
NWB=1
AN=DFLOAT (NNB)
NPT=1
AKS2= (2. DO*PI/ACONST)**2*DFLOAT(KSQ)
IF (NPT.GT.NKPTRK.AND.NSPIN.EQ.2) GDN=GUMDF*GUMEN
IF (NPT.GT.NKPTRK) GO TO 910
GCOLT=VCKO(NPT)+CVKMW(NPT)
IF (NSPIN.EQ.2) G0 TO 910
GEXCH=GECH+DVXCUP(NPT)
G0=GE+DZFUP(NPT)
GUM=GUM+DPUP(NPT)
GO TO 910
910 CONTINUE
GEXUP=VXCUPD(NPT)+DVXCUPD(NPT)
GEXDN=VXCNDO(NPT)+DVXCN(NPT)
GUP=WUD(NPT)+DUF(NPT)
GDN=VXDNO(NPT)+DWD(NPT)
GUP=WIPU(NPT)+DFUF(NPT)
GURB=FDNO(NPT)+DFU(NPT)
DSN=PHBAGA_DIOIA_DEN

GUM=GUM+GUM

914 CONTINUE
IF (NPT.NE.1) GC TO 918
GCOULT=GCOULT
GCOUEL=GCOULT
WRITE (6,856) GCOUEL,GCOULT,VKO(1)

918 CONTINUE
IF (NPT.EQ.1) GC TO 920
GCOULT=GCOULT
GCOUEL=GCOULT+2*DSO*PI/Z/OMEGA/AKS

920 CONTINUE
IF (NPT.EQ.1) WRITE (6,858) GCOUEL,GCOULT
VCESUM=VCESUM*GCOUEL*ANNE
VTSUM=VTSUM*GCOULT*ANNE
VTPSUM=VTPSUM*GCOULT*GUM*ANNE
VPSUM=VPSUM*GCOUEL*GUM*ANNE
IF (NSPIN.EQ.2) GO TO 924
VXCPFSM=VXCPFSM*GEXCH*GUM*ANNE
VXCPDD=VXCPDD*WPSUM
WPSUM=WPSUM+GUM*ANNE
WPDS=WPSUM

924 CONTINUE
IF (NPT.LE.NKPTBN) GC TO 928
VP=VP1=GCOUEL*GUM*ANNE
VP2=VP2=GCOULT*GUM*ANNE
IF (NSPIN.EQ.2) GC TO 923
VXCF1=VXCF1>GEXCH*GUM*ANNE
VXCF2=VXCF1
WT=WT1=GUM*ANNE
WPUD2=WT1

928 CONTINUE
IF (NSPIN.EQ.1) GC TO 930
VXCPUDS=VXCPUDS*GEXUP*GUMUP*ANNE
VXCPDS=VXCPDS*GEXD*GUMD*ANNE
VXCPUD=VXCPUD*VXCPDS
WPUPSM=WPUPSM*GUP*GUMUP*ANNE
WPDNSM=WPDNSM*GWD*GUMDN*ANNE
WPUDS=WPUPSM*WPDNSM
IF (NPT.LE.NKPTBN) GC TO 930
VXCPU1=VXCPU1>GEXUP*GUMUP*ANNE
VXCPD1=VXCPD1>GEXD*GUMDN*ANNE
VXCPD2=VXCPD1+VXCPD3
WPUP1=WPUP1+GNUM*ANNE
WPDN1=WPDN1+GWDN*GUMDN*ANNE
WPUD2=WPUP1*WPDN1

930 CONTINUE
IF (NPT.EQ.1) WRITE (6,948)
IF (NPT.EQ.2) WRITE (6,950)
IF (NPT.EQ.1) CMPT.EQ.2 OR NPT.EQ.300 OR
& NPT.EQ.1000 OR NPT.EQ.1500 OR NPT.EQ.1600 OR NPT.EQ.2000
& WRITE (6,955) NPT,TV1,TV2,VXCP2,WPDL2,VCESUM,VTSUM,VTPSUM,
& VXCPUD,WPDS
GO TO 898

934 CONTINUE
REWOIND 11
IF (ITETCTL.NE.1) GC TO 938
PRELINE 12

938 CONTINUE
VP=VP1*OMEGA/2.0
DSN-PHAGA, DIOLA, DEN

VT = VP2*OMEGA/2.0
VP = VXCP2*OMEGA
W = WPDD2*OMEGA

C
IF (IPTOTL.EQ.2) WP = VP/4.0
C = V2*3.2877*2.0*PI/ACOSST
UNNU = V2*2C/(2.0*DIAM2)
D = 2*VCSUM/2.0*DIAM2/2.0/PI**2
W = VTPSUM*OMEGA/2.0
X = VXCPU*OMEGA
VEPS = VEPSUM*OMEGA/2.0
VECSM = WPDDU*OMEGA
IF (IPTOTL.EQ.2) VECSM = VECSM/4.0

C
CALCULATE THE TOTAL ENERGY

ETOTH = ESNEL + U - EVCSM
EFOTEN = U + E
EKINET = ESNGEL + 2.0*U - X
PRESS = (2.0*EKINET + EPOTEN + 3.0*EVCSM)/(3.0*OMEGA)
IF (NSPIN.EQ.1)
WRITE(6,940)
IF (NSPIN.EQ.2)
WRITE(6,944)

940 FORMAT(/,2X,'NP1',2X,'ESMVP FR40',2X,'ESMVCP FR40',2X,
6.'ESMVX CP FR40',2X,'C=2*PI/A',3X,'UKUC=WUC')
IF (NSPIN.EQ.1)
WRITE(6,950)
WRITE(6,949)

944 FORMAT(/,2X,'NP2',2X,'ESMVP FR40',2X,'ESMVCP FR40',2X,
6.'ESMVX CP FR40',2X,'C=2*PI/A',3X,'UKUC=WUC')
IF (NSPIN.EQ.1)
WRITE(6,950)
WRITE(6,949)

949 FORMAT(/,2X,'NP3',2X,'ESMVP FR40',2X,'ESMVCP FR40',2X,
6.'ESMVX CP FR40',2X,'C=2*PI/A',3X,'UKUC=WUC')
IF (NSPIN.EQ.1)
WRITE(6,950)
WRITE(6,949)

949 FORMAT(/,2X,'NP4',2X,'ESMVP FR40',2X,'ESMVCP FR40',2X,
6.'ESMVX CP FR40',2X,'C=2*PI/A',3X,'UKUC=WUC')
IF (NSPIN.EQ.1)
WRITE(6,950)
WRITE(6,949)

CALCULATE THE DENSITY OF STATES

CONTINUE
IF (NDENS.EQ.0) GC TO 180
EE = EMIN
DC 100 NE = 1, NMAX
EN(NX) = EE
SWUP(NJ) = 0.0
SWDN(NJ) = 0.0
TBUP(NJ) = 0.0
TBDN(NJ) = 0.0
ESNGO(NJ) = 0.0
ESING{NE} = 0 DC
EE=EE+DE
IF (EN(NE).GE.FERM.0R.EE.LE.FERM) GC TO 100
EN(NE) = FERM
100 CONTINUE
DO 118 IT=1, IPTOL
11=IPT(1,IT)
12=IPT(2,IT)
13=IPT(3,IT)
14=IPT(4,IT)
DB(I1) MB=1, NBFERM
E1=EUP(NB,11)
E2=EUP(NB,12)
E3=EUP(NB,13)
E4=EUP(NB,14)

C C
POWELLING STATEMENTS ARE USED FOR SUBROUTINES I7ENST
C C
IF (E1.LE.E2) GC TO 102
101 CONTINUE
EE=E1
E1=E2
E2=EE
IF (E2.LT.E3) GO TO 104
103 CONTINUE
EE=E2
E2=E3
E3=EE
IF (E1.GT.E2) GC TO 101
104 IF (E3.LT.E4) GO TO 105
EE=E3
E3=E4
E4=EE
IF (E2.LT.E3) GO TO 103
105 CONTINUE
EE=E4-E3
IF (D43.LE.ZERO) E4=E4*ZERO
E3=E3-E2
IF (D32.LE.ZERO) E2=E2-ZERO
D2=EE-E1
E1=E1-ZERO
E2=EE-E3
IF (D21.LT.ZERO) E1=E1-2.*E2+200
D1=E1-E2
IF (D21.LT.3.*ZERO) E4=E4+ZERO
E2=EE-E3
IF (E4.LE.E3.OR.E3.LE.E2.OR.D41.LE.E1.LE.30.*ZERO)
C C
IF (NSPIN.EQ.1) GO TO 118
E1=EDB(NB,11)
E2=EDB(NB,12)
E3=EDB(NB,13)
E4=EDB(NB,14)
IF (E1.LE.E2) GC TO 112
111 CONTINUE
EE=E1
E1=E2
DSM=PHBAGA_DJOLA_DEN

112 IF (E2.LT.E3) GO TO 114
113 CONTINUE
E2=E2
E2=E3
E3=E3
IF (E3.GT.E2) GO TO 111
114 IF (E3.LT.E4) GO TO 115
E3=E3
E3=E4
EN=EN
IF (E2.GT.E3) GC TO 113
115 CONTINUE
D3=E4-E3
IF (D4.LE.ZERO) EN=EN+ZERO
D2=E3-E2
IF (D3.LE.ZERO) E2=E2-ZERO
D2=E2-E1
IF (D2.LE.ZERO) E1=E1-ZERO
E4=E3-E4
EN=E4-E1
IF (D4.LT.3.*ZERO) E4=E4+ZERO
C &WRITE({,140}) Figure,E4,EN,NSPIN,SK,DN,NSPIN,SK,DN,NSPIN,SK,DN
CALL TDEST({,120}) EN,NSPIN,SK,DN
CALL TDECT({,120}) EN,NSPIN,SK,DN
118 CONTINUE
IF (NSPIN.EQ.1) GO TO 150
WRITE(6,120)
120 FORMAT(//,6X,'E',10X,'DEN UP',6X,'DEN DOWN',6X,'ELEC UP',7X,'ELEC DOWN',5X,'TOTAL ELEC',7X,'EAG NO',7X,'ESINGLE',/)
DO 130 NE=1,NMAX
EN=E4+TUP(NE)+TWN(NE)
EAG=TUP(NE)+TWN(NE)
ESING=ESINGU(NE)+ESINGD(NE)
IF (DABS(SUP(NE)).GT.ZERO) GO TO 150
&o130 CONTINUE
140 FORMAT(1X,8F14.7)
DO 143 NE=1,NMAX
EN=E4+TUP(NE)
GSUP=SWUP(NE)
GTW=TWUP(NE)
143 WHITE(40,148) GEN,GSUP,GTW
DO 145 NE=1,NMAX
EN=E4+TUP(NE)
GSUP=SWUP(NE)
GTW=TWUP(NE)
145 WRITE(41,148) GEN,GSUP,GTW
148 FORMAT(IF15.5)
GO TO 180
150 CONTINUE
WRITE(6,160)
160 FORMAT(//,11X,'E',10X,'DEN',7X,'ELEC NO',6X,'ESING',/)
DO 170 NE=1,NMAX
EN=E4+TUP(NE)
IF (DABS(SUP(NE)).GT.ZERO) GO TO 150

 RAW TEXT END
DSM=PHBAGA.EIOLA.DEN

&WRITE(6,140) EN(NE),SWOP(NE),TWUP(NE),ESINGU(NE)
GE=EN(NE)
GSWUP=SWOP(N)
GTWUP=TWUP(N)
WRITE (40,148) GE,GSWUP,GTWUP
176 CONTINUE
160 CONTINUE
STOP
END

SUBROUTINE TELC1(E1,E2,E3,E4,CONST,EN,SN,HMAX)

C E1,E2,E3,E4 ARE E(K) AT FOUR CBorners Of Metershedrons.
C SN(NE)/EAVRG IS THE FRACTION OF THE VOLUME WITH E(K).LE.EN(NE).
C TELC1 IS USED FOR CALCULATION OF THE SINGLE ELECTRON ENERGy

IMPLICIT REAL-ST8(A-P,H,0-2)
DIMENSION EN(NMAX),SN(NMAX)
IF (E1.LE.E2) GO TO 20
10 CONTINUE
EE=E1
E1=E2
E2=EE
20 IF (E2.LE.E3) GO TO 40
30 CONTINUE
E1=E2
E2=E3
E3=EE
IF (E1.GT.E2) GO TO 10
40 IF (E3.LE.E4) GO TO 50
E1=E3
E3=E4
E4=EE
IF (E2.GT.E3) GO TO 30
50 CONTINUE
IF (EN(NMAX).LT.E1) RETURN
D41=E4-E1
IF (EN(1).LE.EN) GO TO 70
EAVRG=(E1+E2+E3+E4)/4.DO
DO 60 NE=1,NMAX
60 SN(NE)=SN(NE)*CONST*EAVRG
RETURN
70 CONTINUE
D21=E2-E1
E31=E3-E1
D31=E3-E2
E41=E4-E2
D41=E4-E3
IF (D21.GT.0.DO) CS1=1.DO/(D21*D31*D41)
80 IF (D32.LE.0.DO) GC TO 90
CS23=-1.DO/(D31*D42*D43)/(D41*D32)
CS22=3.DO/(E31*D41)
CS21=D21*CS22
CS20=D21*CS21/3.DO
90 IF (D41.GT.0.DO) CS4=1.DO/(D41*D42*D43)
DO 140 NE=1,NMAX
EE=EN(NE)
IF (EE.LE.E1) GO TO 140
130 CONTINUE
131
END

//LKED.S(XLIB DD DSN=D1103.CALLAWAY.RVCAPLIB,DISP=SHR
// DD DSN=DS103.CALLAWAY.BNDPKG.SUBLIB.COMPL,DISP=SHR
// DD DSN=SYS1.VGATLIB,DISP=SHR
// DD DSN=SYS2.FCRTL1E,DISP=SHR
// DD DSN=SYS2.U5P.LIB,DISP=SHR
// DD DSN=SYS2.PLOT1.LIB,DISP=SHR
//GO.FT10F001 DD UNIT=3380,VCL=SER=USER77,DISP=SHR,
// DCB=(ELKSIZ=7294,RECFM=VS,RECL=00176),
// DSNAM=PBHAGA.DIOLA.FEF5P4.ECC.EAND
//GO.FT11F001 DD UNIT=3380,VCL=SER=USER77,DISP=SHR,
// DSNAM=PBHAGA.DIOLA.FEF5P4.BCC.WK1
//GO.FT12F001 DD UNIT=3380,VCL=SER=USER77,DISP=SHR,
// DSNAM=PBHAGA.DIOLA.FEF5P4.BCC.WK3
//GO.FT4F001 DD UNIT=3380,VCL=SER=USER77,DISP=(NEW,CATLG),
// SPACE=(TRK,(20,10),ELSE),
// DCD=(ELKSIZ=4500,RECFM=FE,RECL=0045),
// DSNAM=PBHAGA.DIOLA.FEF5P4.BCC.DSSTUP3
//GO.FT4F001 DD UNIT=3380,VCL=SER=USER77,DISP=(NEW,CATLG),
// SPACE=(TRK,(20,10),ELSE),
// DCD=(ELKSIZ=4500,RECFM=FE,RECL=0045),
// DSNAM=PBHAGA.DIOLA.FEF5P4.BCC.DSSTUP3
//GO.FT17F001 DD UNIT=3380,VCL=SER=USER77,DISP=SHR,
// DSNAM=PBHAGA.DIOLA.FEF5P4.BCC.SELFVX
//GO.FT27F001 DD UNIT=3380,VCL=SER=USER77,DISP=SHR,
// DSNAM=PBHAGA.DIOLA.FEF5P4.BCC.SELFVX
//GO.FT37F001 DD UNIT=3380,VCL=SER=USER77,DISP=SHR,
// DSNAM=PBHAGA.DIOLA.FEF5P4.BCC.SELFDD
//GO.SYS1K DD *
1 1
901 20 1 2 2 15 0 43 1 40 1
-1.0 0.0025 0.00001 26.0 26.0 5.4057
//
Table 8.1: Valence band energies at high symmetry points of the Brillouin zone of BCC iron -
in Rydbergs (Ry) - for up (+) and down (-) spins. The Lattice constant $a = 5.2$ a.u.

The Fermi energy $E_F = -0.0398$ Ry

<table>
<thead>
<tr>
<th></th>
<th>$\Gamma^+$</th>
<th>$\Gamma^-$</th>
<th>$P^+$</th>
<th>$P^-$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$-0.6971$ (1)</td>
<td>$-0.6811$ (1)</td>
<td>$-0.3071$ (4)</td>
<td>$-0.2186$ (4)</td>
<td></td>
</tr>
<tr>
<td>$-0.2267$ (25')</td>
<td>$-0.1069$ (25')</td>
<td>$-0.3071$ (4)</td>
<td>$-0.2186$ (4)</td>
<td></td>
</tr>
<tr>
<td>$-0.01101$ (12)</td>
<td>$0.0484$ (12)</td>
<td>$-0.0905$ (3)</td>
<td>$0.0727$ (3)</td>
<td></td>
</tr>
<tr>
<td>$-0.0037$ (3)</td>
<td>$0.1455$ (3)</td>
<td>$0.7285$ (15)</td>
<td>$0.7515$ (15)</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>$N^+$</th>
<th>$N^-$</th>
<th>$H^+$</th>
<th>$H^-$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$-0.4429$ (1)</td>
<td>$-0.3635$ (1)</td>
<td>$-0.4354$ (12)</td>
<td>$-0.3300$ (12)</td>
<td></td>
</tr>
<tr>
<td>$-0.3185$ (2)</td>
<td>$-0.2107$ (2)</td>
<td>$-0.4354$ (12)</td>
<td>$-0.3300$ (12)</td>
<td></td>
</tr>
<tr>
<td>$0.0178$ (1)</td>
<td>$-0.0011$ (25')</td>
<td>$-0.0196$ (25')</td>
<td>$0.1198$ (25')</td>
<td></td>
</tr>
<tr>
<td>$-0.0935$ (4)</td>
<td>$0.0419$ (1)</td>
<td>$-0.0196$ (25')</td>
<td>$0.1198$ (25')</td>
<td></td>
</tr>
<tr>
<td>$-0.0153$ (12)</td>
<td>$0.0691$ (4)</td>
<td>$-0.0196$ (25')</td>
<td>$0.1198$ (25')</td>
<td></td>
</tr>
</tbody>
</table>
Table B2. Valence band energies at high symmetry points of the Brillouin zone of BCC iron -
in Rydbergs (Ry) - for up (+) and down (-) spins. The Lattice constant a = 5.4057 a.u.
The Fermi energy \( E_F = -0.1214 \text{ Ry} \)

<table>
<thead>
<tr>
<th></th>
<th>( \Gamma^+ )</th>
<th>( \Gamma^- )</th>
<th>( P^+ )</th>
<th>( P^- )</th>
</tr>
</thead>
<tbody>
<tr>
<td>(-0.7275 \text{ (1)})</td>
<td>(-0.7125 \text{ (1)})</td>
<td>(-0.3551 \text{ (4)})</td>
<td>(-0.2589 \text{ (4)})</td>
<td></td>
</tr>
<tr>
<td>(-0.2863 \text{ (25')})</td>
<td>(-0.1565 \text{ (25')})</td>
<td>(-0.3551 \text{ (4)})</td>
<td>(-0.2589 \text{ (4)})</td>
<td></td>
</tr>
<tr>
<td>(-0.2863 \text{ (25')})</td>
<td>(-0.1565 \text{ (25')})</td>
<td>(-0.3551 \text{ (4)})</td>
<td>(-0.2589 \text{ (4)})</td>
<td></td>
</tr>
<tr>
<td>(-0.2863 \text{ (25')})</td>
<td>(-0.1565 \text{ (25')})</td>
<td>(-0.1729 \text{ (3)})</td>
<td>(-0.0011 \text{ (3)})</td>
<td></td>
</tr>
<tr>
<td>(-0.1880 \text{ (12)})</td>
<td>(-0.0202 \text{ (12)})</td>
<td>(-0.1729 \text{ (3)})</td>
<td>(-0.0011 \text{ (3)})</td>
<td></td>
</tr>
<tr>
<td>(-0.1880 \text{ (12)})</td>
<td>(-0.0202 \text{ (12)})</td>
<td>(0.4931 \text{ (4)})</td>
<td>(0.5605 \text{ (4)})</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>( N^+ )</th>
<th>( N^- )</th>
<th>( H^+ )</th>
<th>( H^- )</th>
</tr>
</thead>
<tbody>
<tr>
<td>(-0.4725 \text{ (1)})</td>
<td>(-0.3870 \text{ (1)})</td>
<td>(-0.4556 \text{ (12)})</td>
<td>(-0.3387 \text{ (12)})</td>
<td></td>
</tr>
<tr>
<td>(-0.3618 \text{ (2)})</td>
<td>(-0.2437 \text{ (2)})</td>
<td>(-0.4556 \text{ (12)})</td>
<td>(-0.3387 \text{ (12)})</td>
<td></td>
</tr>
<tr>
<td>(-0.1889 \text{ (1')})</td>
<td>(-0.0791 \text{ (1')})</td>
<td>(-0.1121 \text{ (25')})</td>
<td>(0.0378 \text{ (25')})</td>
<td></td>
</tr>
<tr>
<td>(-0.1752 \text{ (4)})</td>
<td>(-0.0276 \text{ (1)})</td>
<td>(-0.1121 \text{ (25')})</td>
<td>(0.0378 \text{ (25')})</td>
<td></td>
</tr>
<tr>
<td>(-0.0936 \text{ (3)})</td>
<td>(-0.0038 \text{ (4)})</td>
<td>(-0.1121 \text{ (25')})</td>
<td>(0.0378 \text{ (25')})</td>
<td></td>
</tr>
<tr>
<td>(-0.0927 \text{ (1')})</td>
<td>(0.0595 \text{ (3)})</td>
<td>(0.5863 \text{ (15)})</td>
<td>(0.6086 \text{ (15)})</td>
<td></td>
</tr>
</tbody>
</table>
Table B3. Valence band energies at high symmetry points of the Brillouin zone of BCC iron -

in Rydbergs (Ry) - for up (+) and down (−) spins. The Lattice constant \( a = 5.6 \text{ a.u.} \)

The Fermi energy \( E_F = -0.1017 \text{ Ry} \)

<table>
<thead>
<tr>
<th>( \Gamma^+ )</th>
<th>( \Gamma^− )</th>
<th>( P^+ )</th>
<th>( P^− )</th>
</tr>
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<tbody>
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<td>-0.7286 (1)</td>
<td>-0.3881 (4)</td>
<td>-0.2842 (4)</td>
</tr>
<tr>
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<td>-0.1894 (25')</td>
<td>-0.3881 (4)</td>
<td>-0.2842 (4)</td>
</tr>
<tr>
<td>-0.3291 (25')</td>
<td>-0.1894 (25')</td>
<td>-0.3881 (4)</td>
<td>-0.2842 (4)</td>
</tr>
<tr>
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<td>-0.1894 (25')</td>
<td>-0.2325 (3)</td>
<td>-0.0532 (3)</td>
</tr>
<tr>
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<td>0.0683 (12)</td>
<td>-0.2325 (3)</td>
<td>-0.0532 (3)</td>
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<tr>
<td>-0.2442 (12)</td>
<td>0.0683 (12)</td>
<td>0.3849 (4)</td>
<td>0.4540 (4)</td>
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<td>( N^− )</td>
<td>( H^+ )</td>
<td>( H^− )</td>
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<td>-0.4647 (12)</td>
<td>-0.3355 (12)</td>
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<td>-0.1802 (25')</td>
<td>-0.0204 (25')</td>
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<td>-0.0204 (25')</td>
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<td>-0.0204 (25')</td>
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<td>0.4983 (15)</td>
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Table B.4. Valence band energies at high symmetry points of the Brillouin zone of FCC iron, in Rydberg (Ry), for up (↑) and down (↓) spins. The lattice constant is $a = 6.5516$ a.u. The Fermi energy is $E_F = -0.0573$ Ry

<table>
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<th>$\Gamma_4$</th>
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<th>$X_4$</th>
<th>$W_4$</th>
<th>$W_4$</th>
<th>$L_4$</th>
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<td>-0.1357</td>
<td>-0.3911</td>
<td>-0.3316</td>
<td>-0.2756</td>
<td>-0.2162</td>
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<td>-0.2234</td>
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<td>+0.0873</td>
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<td>+0.1713</td>
<td>+0.6171</td>
<td>+0.6439</td>
<td>3</td>
<td>-0.0317</td>
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<td>$\Gamma_4$</td>
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<td>-0.0960</td>
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Table B.5 Valence band energies at high symmetry points of the Brillouin zone of FCC iron, in Rydberg (Ry), for up (\(\uparrow\)) and down (\(\downarrow\)) spins. The lattice constant is \(a = 6.8107\) a.u. The Fermi energy is \(E_F = -0.1283\) Ry.

<table>
<thead>
<tr>
<th>(\Gamma_\uparrow)</th>
<th>(\Gamma_\downarrow)</th>
<th>(X_\uparrow)</th>
<th>(X_\downarrow)</th>
<th>(W_\uparrow)</th>
<th>(W_\downarrow)</th>
<th>(L_\uparrow)</th>
<th>(L_\downarrow)</th>
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<td>-0.1718</td>
<td>-0.4213</td>
<td>-0.3395</td>
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<td>-0.1022</td>
<td>0.0188</td>
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<td>0.0189</td>
<td>-0.1217</td>
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\(X_\uparrow\) | \(X_\downarrow\)
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<td>-0.3320</td>
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<td>-0.3825</td>
<td>-0.3062</td>
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<td>-0.2458</td>
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<td>-0.1768</td>
<td>-0.0591</td>
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<td>-0.1243</td>
<td>-0.0597</td>
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<td>+0.3315</td>
<td>+0.3767</td>
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Table B. 6. Valence band energies at high symmetry points of the Brillouin zone for FCC iron, in Rydberg (Ry), for up (+) and down (−) spins. The lattice constant is \( a = 7.0 \text{ a.u.} \). The Fermi energy is \( E_F = -0.1501 \text{ Ry}. \)

<table>
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<th>( \Gamma )</th>
<th>( \Gamma )</th>
<th>( X )</th>
<th>( X )</th>
<th>( W )</th>
<th>( W )</th>
<th>( L )</th>
<th>( L )</th>
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<td>−0.3658 (1)</td>
<td>−0.4268</td>
<td>−0.3067 (2)</td>
<td>−0.4877</td>
<td>−0.3904 (1)</td>
</tr>
<tr>
<td>−0.3176</td>
<td>−0.1537 (25')</td>
<td>−0.4453</td>
<td>−0.3090 (3)</td>
<td>−0.3626</td>
<td>−0.2318 (3)</td>
<td>−0.3266</td>
<td>−0.1607 (3)</td>
</tr>
<tr>
<td>−0.3176</td>
<td>−0.1537 (25')</td>
<td>−0.1909</td>
<td>−0.0010 (2)</td>
<td>−0.3626</td>
<td>−0.2318 (3)</td>
<td>−0.3266</td>
<td>−0.1607 (3)</td>
</tr>
<tr>
<td>−0.3176</td>
<td>−0.1537 (25')</td>
<td>−0.1673</td>
<td>+0.0229 (5)</td>
<td>−0.2483</td>
<td>−0.0745 (1)</td>
<td>−0.1846 (3)</td>
<td>−0.1526 (2')</td>
</tr>
<tr>
<td>−0.2447</td>
<td>−0.0633 (12)</td>
<td>−0.1673</td>
<td>+0.0229 (5)</td>
<td>−0.1673</td>
<td>+0.0229 (1')</td>
<td>−0.1846 (3)</td>
<td>+0.0041 (3)</td>
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<tr>
<td>−0.2447</td>
<td>−0.0633 (12)</td>
<td>−0.0183</td>
<td>+0.0368 (4')</td>
<td>+0.3838</td>
<td>+0.4539 (3)</td>
<td>−0.1662 (2')</td>
<td>+0.0041 (3)</td>
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</table>

<table>
<thead>
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<th>( K )</th>
</tr>
</thead>
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<tr>
<td>−0.4123</td>
<td>−0.2850 (1)</td>
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<td>−0.2915</td>
<td>−0.1615 (3)</td>
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<tr>
<td>−0.2326</td>
<td>−0.0537 (4)</td>
</tr>
<tr>
<td>−0.1865</td>
<td>+0.0005 (2)</td>
</tr>
<tr>
<td>−0.2492</td>
<td>+0.3278 (1)</td>
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</table>
Table B.7. Least square fit coefficients, as defined in section D of Chapter 4, for the charge form factors of BCC iron. The lattice constants used are 5.0, 5.4057, and 6.0 in atomic units (a.u.).

<table>
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<th>k</th>
<th>l</th>
<th>m</th>
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<th>$a_{1,k,l,m}$</th>
<th>$a_{2,k,l,m}$</th>
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<tbody>
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<td>0</td>
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Table B.8. Least square fit coefficients, as defined in section D of Chapter 4, for the spin form factors of BCC iron. The lattice constants used are 5.0, 5.4057, and 6.0 in atomic units (a.u.).

<table>
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<th>$a_{1,k,\ell,m}$</th>
<th>$a_{2,k,\ell,m}$</th>
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C.1. Evaluation of the Pressure for a Metal

The expression of the pressure $P$ is, for a paramagnetic substance,

$$3PV = 2E_{ki} + E_{PC} - 3 \int \rho \left( e_{xc} - V_{xc} \right) d^3r$$ \hspace{1cm} C.1.1

where

$$E_{ki} = \sum \int \psi_n^*(\vec{k}, \vec{r}) \left( -\nabla^2 \right) \psi_n(\vec{k}, \vec{r}) \, d^3r,$$ \hspace{1cm} C.1.2

$$E_{PC} = -2Z \sum \int \frac{\rho(\vec{r})}{|\vec{r} - \vec{R}_\mu|} \, d^3r + \int \frac{\rho(\vec{r})\rho(\vec{r}')}{|\vec{r} - \vec{r}'|} \, d^3r d^3r' + \sum \frac{Z_\mu Z_\nu}{|\vec{R}_\mu - \vec{R}_\nu|}$$ \hspace{1cm} C.1.3

$V$ is the crystal volume.

The remaining terms in equation C.1.1 are as defined in Chapter 2. Using equations 1 and 2 and the definitions of $U$ and $D$ in Chapter 2 one readily obtains:

$$T = \sum_n E_n(\vec{k}) + 2U - \sum \rho \, V_{xc} \, d^3r$$ \hspace{1cm} C.1.4

The above expression of $E_{PC}$ yields:

$$E_{PC} = D - U$$ \hspace{1cm} C.1.5

The last term in equation C.1.1 (sign included) in simply $\Delta_{xc}$. We therefore have:

$$3PV = 2 \sum_n E_n(\vec{k}) + 3U + D - 2X + \Delta_{xc},$$ \hspace{1cm} C.1.6
with

\[ x = \int \rho \ V_{xc} \ \text{d}^3 r \quad \text{C.1.7} \]

This expression can be precisely evaluated by the new version of BNDPKG as shown in program Density provided in appendix A.3. As stated above, this new method does not use a Muffin-Tin\textsuperscript{85} or other approximations in obtaining the pressure \( P \).
VITA

Diola Bagayoko, a son of Djigui Bagayoko and Nagnouma Keita, was born on December 12, 1948 in Bamako, Mali. He attended the secondary school of N'Tomikorobougou from 1962 to 1966 and the Prosper Kamara High School from 1966 to 1969, where he majored in mathematics, physics, and chemistry. He majored from 1969 to 1973, in physics and chemistry at the Ecole Normale Superieure de Bamako. Bagayoko earned a national reputation as a good student by systematically holding the 1st rank in his classes from primary school to college.

After two years of teaching physics and chemistry at Askia Mohamed and Sikasso High Schools he enrolled at the American Language Institut at Georgetown University to acquire english proficiency in October of 1975. He earned a Master's degree in physics from Lehigh University in 1978 and joined the group of professor Callaway at Louisiana State University the same year.

A few of the awards and honors Diola Bagayoko accepted include but are not limited to: the Malien Government fellowship from 1966 to 1973, a French government fellowship (Bourse FAC) from 1970 to 1971, Operation Cross-road Africa Award to visit the United States of America in the summer of 1972, a University of Grenoble (France) grant for practical training in the summer of 1973, African graduate fellowship (AFGRAD) offered by the African American Institute, Brandeis and Lehigh Universities from 1975 to 1980, a Physics department teaching assistantship at Louisiana State University from 1978 to 1981 followed by a research assistantship from 1982 to present.
Diola Bagayoko has been holding membership and leadership positions in various student and professional organizations. These include, at the professional level, the American Physical Society (APS), the International Association for the advancement of appropriate technology for developing countries, and, at the social level, the Organization of Lycee Proper Students (President 1968-1969), the Organization of EN Sup Students (public relations officer 1970-1971), the African Student Organization of Louisiana State University (vice-president 1979-1980, president 1981-1982, and 1983 to present), the International Student Association at L.S.U. (vice-president 1980-1981, president 1981-1982).

Bagayoko has been participating in several international physics conferences. Few of those at which he presented a publication are: the APS Annual meeting in New York City (1980), APS meeting in New Orleans, Louisiana in November 1981, the APS annual meeting in Dallas, Texas in March 1982, the Sanibel International symposium in Palm Coast, Florida, in March 1983. Bagayoko delivered invited talks at social conferences on such subjects as world hunger and voluntarism.

He coauthored and/or authored numerous publications in a number of journals (i.e., physics letters, Physical Review and the International Journal of quantum chemistry) on the electronic, magnetic, bulk, optical and other properties of metals as well as computational procedures. Detailed references are available in his Ph.D. dissertation.

Married and father of one, Diola Bagayoko is currently a Ph.D. candidate in physics at Louisiana State University. His present research interests include the electronic energy band theory of metals and related topics, Laser physics, and the search of solution to relativistic quantum mechanical equations.
EXAMINATION AND THESIS REPORT

Candidate: DIOLA BAGAYOKO

Major Field: Physics

Title of Thesis: Electronic Structure of Iron

Approved:

[Signatures]

Major Professor and Chairman

Dean of the Graduate School

EXAMINING COMMITTEE:

[Signatures]

Date of Examination: July 15, 1983