EXCHANGE ENERGY AND MAGNETISM OF RARE - EARTH METALS

A THESIS SUBMITTED TO THE POST GRADUATE SCHOOL OF AHMADU BELLO UNIVERSITY, ZARIA IN PARTIAL FULFILMENT FOR THE AWARD OF THE MASTER OF SCIENCE DEGREE IN PHYSICS.

BY

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FEBUARY, 1997.

DECLARATIONN

This is to certify that :-

(i) The work reported in this thesis was carried out by me, Hamisu Mai-Unguwa at Department of Physics, Ahamadu Bello University, Zaria, Nigeria.

(ii) This thesis has not been submitted in any form to any institution, both establishment or organazation other than Ahamadu Bello University, Zaria, Nigeria, for the award of degree of Master of Science.

(iii) All authors whose works are cited and referenced in this project reports are duly acknowledged.



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CERTIFICATION

This project report, entitled 'Exchange energy and magnetism of Rare Earth metals' meets the regulations governing the award of Master of Science of Ahamadu Bello University, and is approved for its contribution to knowledge and literary presentation.

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DEDICATION

This thesis is dedicated to my Late Father, my mother and my step mother .

ABSTRACT

In our study of Ferromagnetism, we have used the Heisenberg model as a general frame work. The indirect exchange model of Ruthermann - Kittel interaction (originally proposed for atomic nuclei) is applied to the case of Rare - earth Ferromagnetic systems. This exchange energy (between spins) is calculated as a second order perturbation. The behaviour of the Weiss Mean Field (WMF) which is an approximation of the exchange interaction and the energy spectrum of the spin are presented in graphical form.

Calculation of the WMF and the energy against the Fermi Wave Vector (KF) are performed for simple cubic lattice (SC), Body-Centred Cubic lattice (BCC) and Face-Centred Cubic lattice (FCC) configuration along the [100] direction. The results obtained are in good agreement with those found in the literature. The extension to Hexagonal Closed Pack (HCP) which is the common structure in Rare - earth metals is the major contribution of this project. The plots of the WMF and energy against K_F along [100], [110] and [111] directions give regions of positive values, thereby satisfying the main condition for Ferromagnetic properties.

TABLE OF CONTENTS

		PAGE
	Title	(i)
	Declaration	(ii)
	Certification	(iii)
	Acknowledgement	(iv)
	Dedication	(v)
	Abstract	(vi)
	Table of contents	(vii)
	List of Tables	(ix)
	List of Figures	(x)
	CHAPTER ONE	1
1.0	Introduction	1
1.1	Types of Magnetism	2
1.2	Magnetic Order	3
1.3	Ferromagnetic Materials	3
1.4	Ferri-magnetism and Anti-Ferromagnetism	5
1.5	Magnetic Moment of Free Atom (ion)	6
1.6	Magnetic susceptibility	8
1.7	Rare Earth Metals	9
	CHAPTER TWO	11
2.0	Theory of Spins	11
2.1	The Pauli Exclusion Principle	11
2.1.1	Quantum Mechanical Interpretation of Pauli Exclusion Principle	11
2.2	Classification of State of many Electron of Atom	12
2.3	Hund's Rule	13
2.4	Spin Waves	15
2.5	Block $T^{3/2}$ Law	17
	CHAPTER THREE	21
3.0	Spin Interaction Energy	21
3.1	Exchange Interaction	21
3.2	Derivation of Exchange Integral	23

3.3 Heisenberg Hamiltonian (Direct Exchange) 26

3.4 The S-d Interaction 28

3.5 The Molecular Field Approximation 29

CHAPTER FOUR 33

4.0 Magnetism of Rare-earth Metals 33

4.1 Rudermann-Kittel (indirect) Interaction 33

CHAPTER FIVE 40

5.0 Results and Discussions 40

5.1 Ordered Magnetic Materials 40

5.2 Evaluation of Weis Mean Field 43

5.3 Evaluation of Energy 44

5.4 Conclusion 44

6.0 References 47

Appendix I Proof of Geometrical structure factor (S) for HCP 49

Appendix II Tables 51

Appendix III Graphs 76

LIST OF TABLES

TABLES		PAGE
Table1	Values K_F and WMF for Simple cubic lattice	51
Table2	Values K_F and WMF for Body cubic lattice	52
Table3	Values K_F and WMF for Face cubic lattice	53
Table4	Values K_F and WMF for Hexagonal cubic lattice	54
Table5	Values K_F, WMF and Energy for Simple cubic lattice	55
Table6	Values K_F, WMF and Energy for Hexagonal closed packed lattice	61

LIST OF FIGURES

		PAGE
Fig 1.1.(a)	Random Orientation of spins	3
Fig 1.1(b)	Ferromagnetic order of spins	3
Fig 1.1(c)	Anti-ferromagnetic order spins	3
Fig 1.2(a)	Parallel alignment of spins	5
Fig 1.2(b)	Variation of M_s with temperature T	5
Fig 1.2(c)	Variation of 1/x with temperature T.	5
Fig. 1.3	Variation of x with temperature T.	6
Fig. 3.1.1	Combination of Waves for exchange	21
Fig. 3.1.2	Combination of Waves function for Exchange	21
Fig. 3.1.3	Combination of Waves function for Exchange	23
Fig. 4.1.1	The Poles for contour of integration.	36
Fig.A3.1	Graph of WMF versus K_F for Simple cubic lattice.	76
Fig.A3.2	Graph of WMF versus K_F for Body centered cubic lattice.	77
Fig.A3.3	Graph of WMF versus K_F for Face centered cubic lattice.	78
Fig.A3.4	Graph of WMF versus K_F for hexagonal closed pack lattice.	79
Fig.A3.5	Graph of WMF and E(K) versus K_F for Simple cubic lattice.	80
Fig.A3.6	Graph of WMF and E(K) versus K_F for Simple cubic lattice.	81

CHAPTER ONE

1.0 INTRODUCTION

Ferromagnetism is caused by the interaction between spins of electrons called the exchange energy. The exchange energy is the difference between the parallel spin configuration and the anti-parallel spin. When the exchange energy is positive we have ferromagnetism [Mattis, 1967]. Heisenberg Hamiltonian for the spin-spin interaction (for dilute isotropic and equal exchange integral) is

$$H = -\sum_{i \neq j} JS_i \bullet S_j,$$

where J and S are exchange integral and spin respectively, i and j are integers representing the sites. This is a direct interaction between localised state as found in insulators[Mattis, 1965, and Morrish, 1965].

Magnetism cannot be separated from quantum mechanics. Classical systems cannot display magnetic moment even in magnetic fields. The three principle sources of magnetic moment in free atom are spins, orbital angular momentum and the change in the orbital angular momentum induced by the applied field. While spin S and orbital angular momentum L give the paramagnetic contribution to the magnetisation, the change in the angular momentum L gives the diamagnetic contribution. Magnetic moment is associated with unfilled shells because atoms with filled shell have both L and S equal zero [Kittel, 1976].

Para-magnetism (electric Para-magnetism) is found in (i) atoms, molecules and lattice defects which have odd number of electrons (That is total value of spin not equal to zero). Examples Sodium (Na), NO (gas) and $C(C_6H_5)_3$, (ii) free atoms and ions which have a partially filled inner shell. Examples, transition metals, Iso-electronic with transition metals , rare-earth metals, and actinide elements. (iii) Some few compounds with even number of electrons, these includes, oxygen and organic bi-radicals, and (iv) Metals.

Number (ii) and (iv) are the most important and as a result they are the ones given consideration in most of the previous work done on Para-magnetism [Wagner,1972 and Kittel,1976].

1.1 Types of Magnetism

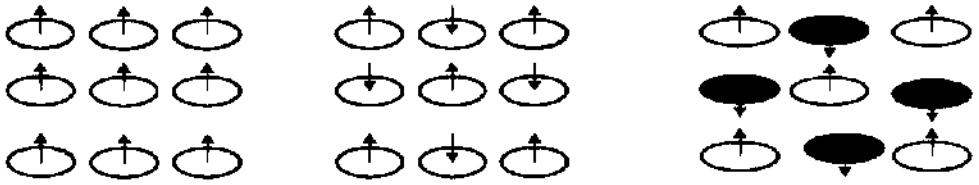
Substances which are maganetised, more or less by a magnetic field are called magnetic substances. All materials, metals, semiconductor and insulators exhibit the phenomenon of magnetism[Animalu,1977]. Each type of magnetism is being characterised by its peculiar properties. Magnetic substances can be classified in terms of the sign and order of magnitude of magnetic susceptibility(χ) which is a parameter characteristic of the substance considered and it is related to the intensity of magnetisation I, and the field H by $I = \chi H$. Generally χ depends on temperature. In this way magnetic substances can be divided into three main classes[Wagner,1972].

Substances which have the value of susceptibility less than zero ($\chi<0$) are called diamagnetic substances. Almost all organic molecules, noble gases, metals, non-metals and superconductors belong to this class. Paramagnetic substances are the one with the value of χ greater than zero($\chi>0$). This class comprises all substances which possess a permanent magnetic moment. These include transition elements of the periodic table, Alkali metals and rare-earth metals. The third class is that of Ferro-magnets. This class has a value of $\chi = \infty$. Or very large. The properties of the Ferro-magnets is linked with definite crystalline structures. So that this class comprises of solids only[Pedersen, 1991].

We can also classify each type of magnetism in terms of magnetic order. In this respect magnetism can be divided into two main classes. These classes are that of ordered and disordered magnetism. Disordered magnetism contain dia-magnetism and Para-magnetism. Ordered magnetism include Ferro-magnetism, Ferri-magnetism, anti-ferromagnetism and Heli-magnetism. These classes differ only in response to the magnetic field[Ododo,1994].

1.2 Magnetic order

Magnetic Ordering provides a means by which three different subclasses of magnetic materials called Ferro-magnets, anti-Ferro-magnets and Ferri-magnets can be distinguished at low temperature[Prentice, 1977]. All these classes belong to a paramagnetic material. Magnetic order is the alignment of spontaneous atomic or molecular moments with respect to one another and with respect to the crystallographic axes. The three case are illustrated in Fig 1.1(c).



(a) Ferro-magnetic (b) Anti-Ferromagnetic (c) Ferri-magnetic

Fig 1.1

Each arrow indicates a magnetic moment and its orientation. Ferro-magnets consist of parallel alignment of all the atomic moments in a crystal as in Fig. 1.1 (a). Anti-ferromagnetic order consists of two likes ferromagnetic arrays of atomic moment directed opposite to one another as shown in Fig. 1.1 (b). Ferri-magnetic order consist of two unlike ferromagnetic arrays that, through coupled anti-parallel, gives a net spontaneous magnetisation in Figure 1.1(C) because of two un-equal magnetic moments of the arrays.

1.3 Ferromagnetic Materials

Ferromagnetic Materials possess atomic magnetic moments which are ordered (aligned) below some critical temperature. If a piece of iron is examined at room temperature it may be found to be in an un-magnetised state. When placed in a weak magnetic field a magnetic moment will be induced. Ferromagnetic materials exhibit spontaneous magnetisation which is spontaneously present within the domains when no field is applied externally... The spontaneous magnetisation which is temperature dependent has its large value at absolute zero and becomes zero at Curie temperature T_C. The magnetisation of a single crystal in an

increasing field differs according to the orientation of the field with respect to the crystal axes. Some directions are directions of easy magnetisation and others are hard direction [Wagner, 1972]. For example in iron(Fe), the cube direction [100] is easy while the direction of the cube diagonal [111] is hard. This is what is called magnetic crystalline anisotropy. Measurements of magnetic crystalline anisotropy give the basic information on the nature of the magnetic atoms. It plays a very important role in determining the thickness, energy and mobility of domain boundary walls. As the temperature increases, the spins become disordered gradually by thermal agitation. This results in the decrease of the spontaneous magnetisation and vanish at Curie temperature T_C. It has been found that at low temperature the decrease of spontaneous magnetisation for iron (Fe) is less than or equal ($\leq$) 2%. The exact form of the decrease is used for distinguishing one theoretical model from the other. For example it can be used to distinguish mean field theory and spin-wave theory[Chicazumi, 1994].

Transition from Ferro-magnet to paramagnet occurs above the Curie temperature but with a magnetic susceptibility that obeys a Curie - Weiss law;

$$\chi = C/(T - T_C)$$

The common examples of Ferro-magnets include:

(i) ion-group series: Fe, Co, Ni

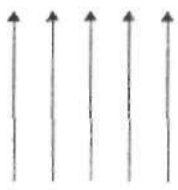
(ii) Rare - earth metals: Gd, Tb, Dy, Ho, Er, Tm.

(iii) CrO_2, $CrBr_3$ EuO, $GdCl_3$ and

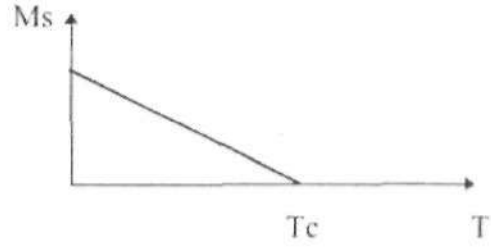
(iv) The alloys of number (i) and (ii) and some alloys of non - magnetic metals e.g Au_4V and $ZnZr_4$.

A piece of a ferromagnetic substance has no net magnetism in the absence of external field in spite of the spontaneous magnetisation within the domains along a given direction. This is due to the existence of regions of spontaneous magnetisation, called domains. The domain magnetisation varies from one domain to another and give zero net magnetisation. When a magnetic field is applied one gets,(i) Growth of Favoured domains at the expense of

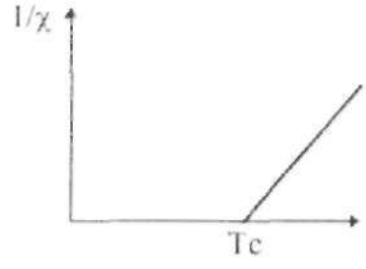
others and (ii) Rotation of the direction of the domain magnetisation to that of the ordered field. This results in a new magnetisation. This is due to the fact that Ferromagnetic substances possesses atomic magnetic moments which are ordered below some critical temperature [Kittel,1976]. Ferromagnetic substances exhibit hysteresis because the process of magnetisation is partly irreversible. On decreasing the field extended to zero there is some remnant magnetisation which is reduced to zero by applying a (negative) coercive field.



Ferromagnetic Ordering of spins (a)



Variation of M_S with Temp. (b)



(c) Variation of $1/\chi$ with temp.

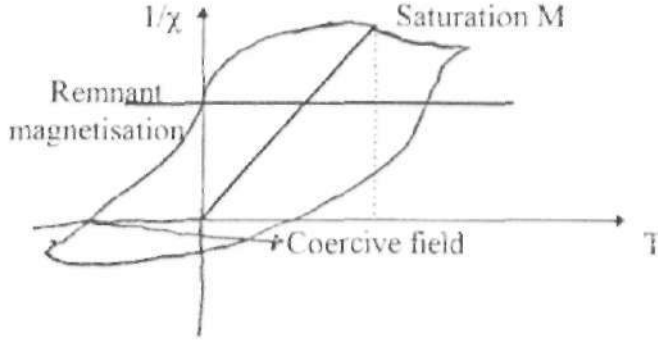


Fig. 1.2

1.4 Ferrimagnetism and Antiferromagnetism

Like Ferro-magnets, Ferri-magnets also show a spontaneous magnetisation below a critical temperature T_N. They also show remenance and other properties similar to Ferro-magnets [Kittel,1976 and Elliot, 1974]. The observed differences are summarised below.

(a) Spontaneous magnetisation M_S verses temperature curves show a greater variability of shape than that of Ferro-magnets.

(b) The value of spontaneous magnetisation is less than the expected one for a full parallel alignment of magnetic dipole.

(c) The Curie - Weiss law is obeyed above T_N but with a negative Weiss constant. that is, $\chi = C/(T + T_N)$

Anti-Ferromagnetic substance consists of two or more interpenetrating ordered sub-lattices each spontaneously magnetised in such a way that the net magnetisation over all sub-lattices is zero. Anti-ferromagnetism is found in ionic compound. For example in fluorides and oxides of Fe - group elements and in Cr, Mn γ-Fe and a few of their alloys (e.g Fe_3Mn, CrPt) and ordered Pt_3Fe.

An important characteristic of anti-Ferro-magnet is that, the susceptibility (as a function of temperature) exhibits a maximum as in Fig.1.3 because of ordering at T_N (the Neel temperature) offsets the decreasing effect of the thermal motion and reduces the responses of the individual dipoles. Also χ is an-isotropic below T_N and field dependent. Above Neel temperature T_N, χ obeys Curie-Weiss law as in ferri-magnetes.

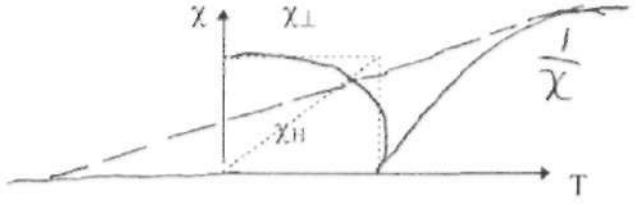


Fig 1.3

T_C is the temperature below which ferromagnetic ordering is effective. T_N negative is the temperature above which Anti-ferromagnetism is effective.

1.5 Magnetic Moment of free atom (ion)

Free ions exist in stationary states characterised by definite values of the orbital, spin, total and z-component of total angular momentum quantum numbers L, S, J and J_Z respectively. When the applied field is in the z- direction and is small. The above operators commute with the magnetic field H and with one another [Prentice Hall, 1977].

The total magnetic moment $\mu = -\mu_B (L+2S)$. But μ is not a constant of motion so it can not determine the energy of the ion in a magnetic field. Only the component of μ parallel to J say μ_J can determine the energy of the ion in the magnetic field. Therefore

$$\mu J = - \mu_B (L+2S)\bullet(L+S)$$

$$= -\mu_B(L^2+2S^2 + 3L\bullet S) = - \mu_B (-\tfrac{1}{2}L^2+\tfrac{1}{2}S^2+3/2J^2) \quad .. \qquad (1.5.1)$$

But $J^2 = j(j+1)$; $S^2 = s(s+1)$, and $L^2 = l(l+1)$ . .... (1.5.2)

Therefore

$$\mu\bullet J = -\mu_B \{(3/2j(j+1)-\tfrac{1}{2}l(l+1)+\tfrac{1}{2}s(s+1)\}$$

But $\mu\bullet J = \mu J$, therefore

$$U_J = g\mu_B J$$

Therefore

$$\mu\bullet J = g\mu_B J^2$$

$$\mu J = - \mu_B\{3/2j(j+1)-\tfrac{1}{2}l(l+1)+\tfrac{1}{2}s(s+1)\} \quad ..... \qquad (1.5.3)$$

have a definite value.

The Lande g-factor or spectroscopic splitting factor g is defined as

$$g = \frac{<\mu\bullet J>/\mu_B}{J^2} \quad ..... \qquad ...(1.5.4)$$

$$= 3/2 + \frac{s(s+1)-l(l+1)}{j(j+1)}$$

we can see that if $L = 0$,then $g = 2$; and if $S = 0$, then $g = 1$

This means that in the presence of a field B (along the Z - axis say) one gets a discrete set of energy levels

$$E_B = - \mu_J\bullet B = - g\mu_B M_J B \quad ..... \qquad (1.5.5)$$

Where M_J takes the value (2j+1) from -J to + J

1.6 Magnetic Susceptibility

Consider a non-interacting system which can therefore be described by Hamiltonians consisting of the sum of the individual terms. If the static susceptibility is obtained by determining the response of the system to a perturbation by a time-independent magnetic field B . If the non-interacting system are identical and in the absence of an external field each atom has a corresponding Hamiltonian H^0_i to which a Zeeman term H_i^Z is added when a field is applied[Crangle, 1977]. Thus

$$H_{system} = \sum_{i=1}^{N} H_i \; S \sum_{i=1}^{N} (H_i^0 + H_i^Z) \qquad (1.6.1)$$

$$\text{but } H_i^Z = \mu_B(L + 2S)\bullet B + (e^2/8m) \sum_{\alpha=1}^{S} (B \times r_\alpha)^2 \qquad (1.6.2)$$

When we assume that there are S electrons in the i^{th} ions the magnetic moment operator is defined as

$$M = -\partial H/\partial B$$

$$= -\mu_B(L + 2S) - e^2/4m \sum_{\alpha=1}^{S} \{r_\alpha^2 - (r_\alpha \bullet B) r_\alpha\} \qquad (1.6.3)$$

If B is in the J direction

$$M = -\mu_B(L + 2S) - (e^2/4m) \sum_{\alpha=1}^{S} \{(x_\alpha^2 + y_\alpha^2 + z_\alpha^2) - B z_\alpha \bullet r_\alpha\} \qquad (1.6.4)$$

and the z-component of the magnetic moment is

$$M_Z = \langle M \rangle_Z = -\mu_B \langle L_Z + 2S_Z \rangle - (e^2/4m) \left\langle \sum_{\alpha=1}^{S} x_\alpha^2 + y_Z^2 \right\rangle$$

$$= S\langle \mu_Z^p \rangle + \langle \mu_Z^d \rangle \qquad (1.6.5)$$

The magnetic part of the energy of the system has expectation value

$$E_B = \mu_B \langle (L + 2S)\bullet B \rangle + (e^2/8m) \left\langle \sum_{\alpha=1}^{S} (B x r_\alpha)^2 \right\rangle \qquad (1.6.6)$$

For B along the z-axis, we have

$$E(B) = \mu_B B \langle (L_Z + 2S_Z) \rangle + (e^2 B^2/2m) \left\langle \sum_{\alpha=1}^{S} (x_\alpha^2 + y_\alpha^2) \right\rangle$$

$$S \langle \mu_z^p \rangle B - \tfrac{1}{2} \langle \mu_z^d \rangle B \qquad (1.6.7)$$

The first term in the above equation gives the permanent magnetic moment and is responsible for paramagnetism. The second term is responsible for diamagnetism.

However, if eigen values $E_J(B)$ of the Hamiltonian are evaluated to the second order in perturbation theory, it is obtained that

$$E_J(B) = E_j^o - \mu_{jj} B - \sum_n \frac{|\mu_{nj}|^2 B^2}{E_n^o - E_j^o} + (e^2 B^2/8m) \left\langle \sum_\alpha (x_\alpha^2 + y_\alpha^2) \right\rangle \qquad (1.6.8)$$

where $\mu_{nj} = \langle \psi_n | \mu_z^p | \psi_j \rangle$ and ψ_n, ψ_j are the unperturbed wave function of the ion. The average magnetic moment on the j^{th} ionic state along B is given by

$$M_j = - \partial \langle H \rangle / \partial B$$

$$= \mu_{jj} + \sum_n \frac{2 |\mu_{nj}|^2 B}{E_n^o - E_j} - (e^2 B/4m) \left\langle \sum_\alpha (x_\alpha^2 + y_\alpha^2) \right\rangle$$

$$= \mu_{jj} + 2 |\mu_{joj1}|^2 B - (e^2 B/4m) \left\langle \sum (x_\alpha^2 + y_\alpha^2) \right\rangle \qquad (1.6.9)$$

As before the first term is responsible for Para-magnetism and the third term is responsible for dia-magnetism. The second term which is important only if $(E_n^o - E_j)$ is not large is what give rise to the so called Van Vleck para-magnetism[Vonsovseki, 1971].

1.7 Rare -Earth Metals (REM)

The REM have similar chemical properties. This is because of their identical electronic configuration ($5s^2 5p^6$). In addition to the above the influence of high energy state is negligible. The magnetic behaviour of a particular rare-earth metal depends on the number of electrons in the 4f shell. In-fact what distinguishes the magnetic behaviour of one metal species from the other is the number of electrons compacted in the inner 4f shell. It is due to this inner unfilled 4f shell that indirect interaction is present in addition to the direct interaction. Use is made of the indirect exchange theory to display the ferromagnetic behaviour of rare-earth metals.[Mattis, 1981]

In dilute solid solutions of a magnetic ion in a non-magnetic metal crystal (such as Manganese(Mn) in Copper(Cu)) there is exchange coupling between the ions and the conduction electrons. The conduction electron is magnetised and this magnetisation causes an indirect interaction between the magnetic ions because the second ion perceives the magnetisation induced by the first ion. This interaction is known as the Ruderman- Kittel interaction(R-K)[Ododo, 1994] It also plays a role in the magnetic spin order of the rare-earth metals[Morris,1965] where the spin of the 4f ions core are coupled together by the magnetisation induced in the conduction electron gas[Rado Suhl,1966].

The aim of this work is to obtain a suitable expression from the R-.K theory and use computer to analyse the character of the indirect exchange. We would also display the Weiss Mean Field WMF and the Magnon energy E(k) Spectrum.

CHAPTER TWO

2.0 THEORY OF SPINS

2.1 The Pauli Exclusion Principle

In the absence of spin-orbit coupling the behaviour of the electron is described by specifying the values of its four quantum numbers(n,l,m_l,m_s) that are respectively the principle quantum number, the orbital quantum number, the z-component of the orbital quantum number and the z-component of the spin quantum number. The Pauli exclusion principle states that no two electrons can have the same set of quantum numbers (n,l,m_l,m_s). The lowest energy or the ground state electron configuration for many electron atoms can be explained using Pauli exclusion principle together with atomic shell model. Magnetism can not be separated from quantum mechanics[Blakemore, 1983]. The three principle sources of magnetic momentum are the spin, the orbital angular momentum and the change in the orbital moment induced by applied field as a result of Pauli principle and Hund's rule.

2.1.1 Quantum Mechanical Interpretation of Pauli Exclusion Principle

Consider two non-interacting, identical indistinguishable particles in states $\psi_a(1)$ and $\psi_b(1)$, so that the total wave function $\psi_{ab}(1,2)$ is given by

$$\psi_{ab}(1,2)= \psi_a(1)\psi_b(2) \qquad (2.1.1)$$

If the position of the two particles are interchanged the new wave function is $\psi_{ab}(2,1) = \psi_a(2)\ \psi_b(1)$. but since the two particles are the same (identical), exchanging their positions does not change their probability. Thus[Crangle, 1977 and Schiff, 1968],

$$|\psi_{ab}(2,1)|^2 = |\psi_{ab}(1,2)|^2 \qquad (2.1.2)$$

This means that either the wave function is symmetric if

$\psi_{ab}(2,1) = +\psi_{ab}(1,2)$ or is antisymmetric if

$$\psi_{ab}(2,1) = -\psi_{ab}(1,2) \qquad (2.1.3)$$

Thus both $\psi_{ab}(2,1)$ and $\psi_{ab}(1,2)$ are the eigen functions of the system and so are their linear combinations, resulting in the symmetric wave-functions ψ_s given by

$$\psi_S = 1/\sqrt{2}[\psi_{ab}(1,2) + \psi_{ab}(2,1)] \quad \text{symmetric} \quad (2.1.4)$$

and $$\psi_A = 1/\sqrt{2}[\psi_{ab}(1,2) - \psi_{ab}(2,1)] \quad \text{anti-symmetric} \quad (2.1.5)$$

Both the symmetric wave-function ψ_S and anti-symmetric wave-function ψ_A are solutions of the Schrödinger equation corresponding to the same energy, but quantum theory cannot tell whether the total wave-function is symmetric ψ_S or anti-symmetric ψ_A. Now suppose we try to put both particles in the same state, that is $\psi_a = \psi_b$, then the anti-symmetric wave function takes the form

$$\psi_A = 1/\sqrt{2}[\psi_{aa}(1,2) - \psi_{aa}(2,1)]$$

$$= 1/\sqrt{2}[\psi_a(1)\psi_a(2) - \psi_a(2)\psi_a(1)] + 1/\sqrt{2}[\psi_a(1)\psi_a(2) - \psi_a(1)\psi_a(2)] = 0 \quad (2.1.6)$$

Thus for the anti-symmetric wave function to be non-zero a must not be equal to b($a \neq b$). Thus electron cannot occur in the same quantum state. Hence we can restate the Pauli exclusion principle: the eigen-function of a system containing several electrons or particles with half integral spin must be anti-symmetric.

2.2 Classification of States of Many-Electron of Atom

The quantum numbers (n,l) serve to specify the configuration of an N-electron atom. For example,

$$\text{Cobalt(Co)} = 1s^2 2s^2 2p^6 3s^2 3p^3 3d^7 4s^2$$

In any filled shell the resultant spin and orbital angular momentum S and L are both zero. This is because of the fact that in a filled shell electrons take all allowed value of m_S and m_l. That is to say for any electron with $m_l = m_j$ say, there exists another one with $m_l = -m_l$. Also for any electron with $m_S = m_{½}$ there exists another with $m_S = -m_{½}$. Thus, only the electron outside the filled shells of an atom contribute to its angular momentum.

Eigen states of a many-electrons atom are labelled by the quantum number $|L,S,m_j,m_S\rangle$. The energies of these states are separated by the electron-electron interactions. The variation of the one electron energies with the orbital quantum number L is due to the effective central field.

$$U(r_i) = \sum_{i \neq j} \frac{e^2}{4\pi\epsilon_o} \int \left| \frac{\psi_j(r_{ij})}{r_{ij}} \right|^2 dr_j \quad , \quad \text{central potential} \qquad (2.2.1)$$

while the residue field

$$H_{cor} = \sum_{i>j=1} \left\{ \frac{e^2}{4\pi\epsilon_o r_{ij}} - U(r_i) \right\} \qquad \text{non central potential} \qquad (2.2.2)$$

is responsible for splitting of states with different values of L and S. In the absence of spin-orbit coupling the same (L,S) states are degenerate. Each group of states is called a term or multiplet and is labelled by one of the letters

s p d f g h - - - - -

L = 0 1 2 3 4 5 - - - - -

respectively. The application of the paramagnetic susceptibility formula is dependant on a knowledge of the mutual orientation of the spin $S = \sum s_i$ and orbital momenta $L = \sum l_i$ for a many-electron system in its ground state which is (2J+1) fold degenerate. The mutual orientation is determined by the Pauli exclusion principle, the Coulomb electron-electron interaction and the spin-orbit coupling L•S (Russell-Saunders).

Among the terms designated in spectroscopy by (2s+1) with s p d f g h corresponding to l=0, 1, 2, 3, 4, 5, ... the term that represent the lowest energy which is the ground state is the one determined by Hund's rule.

2.3 Hund's Rule

These are empherical rules derived from spectroscopic data which enables the ground state of an atom or ion to be determined. The only alternative to this rules is the Hartree-Fock self-consistent field method which is very long and cumbersome. The Hund's rules for an electron in a given shell of an atom stated that electrons will occupy orbital in such a way that the ground state is characterised by the following[Kittel, 1976]:

Rule 1: Electrons fill up the 2(2l+1) states of a shell in such a way as to maximise the total spin S. That the maximum value of the total spin S allowed by Pauli exclusion principle.

Rule 2: L takes the maximum value compatible with S, in other words, the maximum value of the orbital angular momentum L with this value of S.

Rule 3: The value of the total angular momentum

$J = |L - S|$ when the shell is less than half-filled

$= |L + S|$ when the shell is more than half-filled

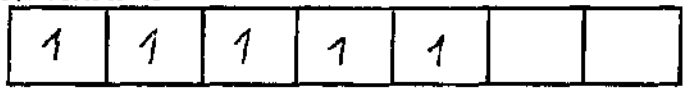
= S when the shell is just half filled, that is, l=0.

The above values, which are due to the consideration of the energies of the coupling mechanisms in descending order(spin-spin, orbit-orbit, total spin-total-orbit) can be explained as follows: Rule 1 is telling us that the spin of the electrons are arranged so that as many of them as possible are parallel to each other with out violating Pauli principle (i.e. only 2 electrons to each value of m). Taking s = +½ for spin up and s = -½ for spin down, then the combined spin angular momentum $S=\sum s_i$ is calculated. Rule 2 is saying that the electrons with spins assigned as in rule 1 are divided amongst the possible values of m. So that $\sum m$ which is combined orbital angular momentum L is maximum. Then we calculate the value of J as in the last rule. For example Sm^{3+}, the configuration is

$$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 4d^{10} 4f^5 5s^2 5p^5$$

The state of concern is $4f^5$

$4f^5 =$



m_l = +L to -L = 3,2,1,0,-1,-2,-3. Applying Hund's rules:

1. $\sum s = ½+½+½+½+½ = 5/2$
2. $\sum m_l = 3+2+1+0-1 = 5$
3. Since f shell takes up 14(maximum) and we have only 5, this is less than half filled, therefore $J = |L - S|$. But $L=\sum l_i=3+2+1+0-1=5$, therefore $J = 5-(^5/_2) = {}^5/_2$ and the representation of the state is $^{2(s+1)}L_J = {}^6H_{5/2}$

2.4 Spin Waves

There are some similarities between excited states of the spin system and those of an elastic solid. If an atom is displaced from its equilibrium position it will oscillate and there are normal modes associated with the crystals. The spins are pointing the same direction in the ground state of Ferro-magnet. The lowest excited state corresponds to the deviation of just one spin from the preferred direction. Since the spin interacts with the other spin on the neighbouring atoms. The effect will propagate in the form of wave through all the other spins. The quanta of this spin wave are called the magnons. In the long wave limit the magnons correspond to the classical wave of the magnetisation in the crystal[Kittel,1976 and White, 1983].

The Hamiltonian of a system of N spins in an external field H which is parallel to the Z-axis is

$$H = g\mu_B H\sum_{i=1} S_{iz} - \sum_{i,j=1} J_{ij}(S_i \bullet S_j) \qquad (2.4.1)$$

Using $S^{+}_i = S_{ix} \pm iS_{iy}$ we have the commutation relation of spin components as

$$[S^{+}_i, S^{-}_j] = 2S_{iz}\delta_{i,j}\,, \quad [S_{iz}, S^{\pm}_j] = \pm S^{\pm}_i \delta_{i,j} \qquad (2.4.2)$$

where δ is a delta function. For convenience we use the Fourier transformed quantities

$$S^{+}_i = \sum_K S^{+}_K \exp(\pm i(k \bullet r_i)), \quad S_{iz} = \sum_K S_{zK} \exp(-i(K \bullet r_i)) \quad \text{and}$$

$$J_{ij} = J(|r_i - r_j|) = \frac{1}{N}\sum_K j_K \exp(i(\mathbf{K} \bullet (r_i - r_j))) \qquad (2.4.3)$$

where K is the vector in the reciprocal lattice and lie in the first Brillouin zone(there are N different K vectors). The inverse of equation (2.4.3)are

$$S^{+}_K = \frac{1}{N}\sum_{i=1}^{N} S^{+}_i \exp(\pm i(\mathbf{K} \bullet r_i))$$

$$S^{z}_k = \frac{1}{N}\sum_{i=1}^{N} S_{iz} \exp(i(\mathbf{K} \bullet r_i)) \qquad (2.4.4)$$

$$J_K = \sum_{i=1}^{N} J(r_i)\exp(-i(\mathbf{K}\bullet\mathbf{r}_i)$$

But the exchange integrals $J(r_i)$depend only on the distance and vanish if referred to one and the same atom, we have

$$J_K = J_{-K} \qquad \text{and} \qquad \sum_K J_K = 0$$

The commutation relation according to the Fourier transform operators are by using equation (2.4.3) and (2.4.4)

$$[S^{+}_K, S^{-}_K] = \frac{2}{N} S^Z_{K-K'} \, , [S^Z_K, S^{\pm}_K] = \frac{\pm 1}{N} S^{\pm}_{K'\pm K} \qquad (2.4.5)$$

The Hamiltonian of equation (2.4.1) can be written as

$$H = g\mu_B H\sum_{i=1}^{N} S_{iZ} - \sum_{i,j=1}^{N} J_{ij}(S_i \bullet S_j)$$

$$= g\mu_B H\sum_{i=1}^{N} S_K{}^Z \exp(-i(K\bullet r_i)) - \sum_{i,j=1}^{N} \frac{1}{N}\sum_K J_K \exp(i(K\bullet r_i - r_j))\sum_K S^Z{}_K \exp(-i(K\bullet r_i)) \bullet S_j$$

$$= g\mu_B H\sum_{i=1}^{N} S^Z{}_K \exp(-i(K\bullet r_i) - \frac{1}{N}\sum_K J_K \sum S_K \exp(i(K-K')(r_i{}^2 - r_{ij})))S_j$$

$$= g\mu_B H\, S_Z{}^\circ - N\sum J_K(S_K \exp(i((K-K')\bullet(r_i{}^2 - r_{ij}) \cdot S_j$$

$$= g\mu_B H S_Z{}^\circ - N\sum_K J_K(S^Z{}_K S^Z{}_{-K} + S^+{}_K S^-{}_K) \qquad (2.4.6)$$

where $S_Z{}^\circ = \sum_{i=1}^{N} S^Z{}_K \exp(i(K\bullet r_i))$ and we use

$$\sum_{i=1}^{N} \exp(i(K\bullet r_i)) = N\delta_{K,0}$$

All moments are parallel to the field in the ground state. If we denote the ground state vector by $|0\rangle$, we can write

$$S_{iZ}|0\rangle = -S|0\rangle \text{ and } S_K{}^Z|0\rangle = -S_K{}^Z|0\rangle_{K,0} \qquad (2.4.7)$$

we can also have $S^-_i|0\rangle = 0$ and $S^-_K|0\rangle = 0$ because of equation 2.4.3. Then we can write the ground state energy as

$$E_0 = -Ng\mu_B SH - NS^2J_0 \qquad (2.4.8)$$

we can show that $S^+_K|0\rangle$ are eigen state of the Hamiltonian. These states are called spin-wave states. These are the corresponding magnetisation wave in the spin systems.

2.5 Bloch $T^{3/2}$ Law

The number of spin wave quanta(magnons) in the spin wave approximation at the temperature T is given by

$$n_K = 1/(\exp(\beta\varepsilon_K) - 1), \quad \text{where } \beta = 1/(KT) \qquad (2.5.1)$$

Each excited spin wave is connected with a change of magnetization by $g\mu_B$. The magnetization of a system at a temperature T is given by

$$M(T) = \vec{M}(0) - \sum_K g\mu_B \bar{n}_K \qquad (2.5.2)$$

where $\vec{M}(0) = Ng\mu_B S$

The mean energy is thus given by

$$E = E_0 + \sum_K \varepsilon_K \bar{n}_K \qquad (2.5.3)$$

The sum is calculated by making a definite choice for exchange interaction. Let us assume the nearest neighbour (n.n) interaction [Mattis, 1967] and let Z be the number of n.n and J the exchange integral between two neighbouring atoms. Then according to equation (2.5.3) we have[Mattis,1981]

$$J_0 = Z_J, \qquad (2.5.4)$$

and

$$J_K = J\sum_\sigma \exp(i(K\bullet\sigma)) \qquad (2.5.5)$$

The sum is over all n.n of the atoms considered and it depends on the lattice structure. Restricting our-self to the cubic crystals, the position of the n.n of atom placed at the origin for S.C. crystal is given by the following six vectors:

l(l,0,0), l(-1,0,0), l(0,+1,0), l(0,-1,0) l(0,0,1) l(0,0-1) ≡ l(±1,0,0), l(0,±1,0), l(0,0,±1),

where l = length of an edge of the elementary cell. For B.C.C crystal the position of the eight n.n are given by the vectors

$$\tfrac{1}{2}l(\pm 1, \pm 1, \pm 1)$$

and F.C.C crystal the 12 vectors are

$$\tfrac{1}{2}l(0,\pm 1, \pm 1,) \tfrac{1}{2}l(\pm 1,0,\pm 1), \tfrac{1}{2}(\pm 1,\pm 1,0).$$

Thus we have $J_O - J_K = ZJ - J\sum_{\sigma} e^{-i(k.\sigma)}$

$$= J\{Z - \sum_{\sigma} e^{-i(k.\sigma)}\} \qquad \text{for S.C. } Z = 6$$

$$= J\{6 - \sum_{l} e^{-i(k.l)}$$

or

$$J_O - J_K = 2J(3 - \cos lk_x - \cos lk_y - \cos lk_z) \text{ for S.C crystal}$$

For B.C.C

$$J_O - J_K = 8J(1-\cos\frac{lk_x}{2}\cos\frac{lk_y}{2}\cos\frac{lk_z}{2}) \qquad (2.5.6)$$

For F.C.C

$$J_O - J_K = 4J(3- \cos\frac{lk_x}{2}\cos\frac{lk_y}{2} - \cos\frac{lk_y}{2}\cos\frac{lk_z}{2} - \cos\frac{lk_x}{2}\cos\frac{lk_z}{2}) \qquad (2.5.7)$$

The spin -wave energy is small for K = 0 and increases according to the above equation almost qua-dratically with wave vector. We restrict ourselves to a long wave length at low temperature and expand E_K in terms of K. According to the above equation we have

$$E_K = g\mu_B H + 2SJl^2K^2 \qquad (2.5.8)$$

For the 3 cubic lattices changing from sum to integral

$$\sum \rightarrow \frac{V}{(2\pi)^3} \int d^3k \qquad (2.5.9)$$

And using equation (2.5.2) after integrating over the angles becomes

$$M(T) = M(0) - \frac{g\mu_B V}{(2\pi^2)} \frac{\int_0^\infty K^2 dK}{\exp(2s\beta J l^2 K^2) - 1} \qquad (2.5.10)$$

We have extended the level of K to ∞ because at low temperature only the long wavelength contributes to the integral. The integral above can be evaluated as

$$\int_0^\infty \frac{K^2 dK}{\exp(\alpha K^2)-1} = \sum_{n=1}^{n} \int_0^\infty K^2 \exp(-n\alpha K^2) dK$$

where $\alpha = 2s\beta J l^2$

$$= \frac{\sqrt{\pi}}{4} \sum_{n=1}^{\infty} \frac{1}{(n\alpha)^{3/2}} = \frac{\sqrt{\pi}\, Z(3/2)}{4\alpha^{3/2}} \qquad (2.5.11)$$

where Z(3/2) is called the Riemann Zeta function. $Z(3/2) \approx 2.612$.

Thus we obtain for the magnetisation

$$M(T) = M(0) - \frac{g\mu_B V}{(2\pi^2)} \cdot \frac{\sqrt{\pi} Z(3/2)}{4\alpha^{3/2}}$$

$$= M(0) - g\mu_B \frac{V}{(2\pi)^2} \cdot \frac{\pi}{4} \cdot \left[\frac{KT}{2sJl^2}\right]^{3/2}$$

$$= M(0) - \frac{M(0)}{S} \cdot \frac{V}{2^4} \frac{1}{\pi^{3/2} l^3} \left[\frac{KT}{2SJ}\right]^{3/2} Z(3/2)$$

$$= M(0) - \frac{M(0)}{Sv} \cdot \left[\frac{KT}{8\pi SJ}\right]^{3/2} Z(3/2)$$

$$= M(0)\left[1 - \frac{1}{vs} \cdot \left[\frac{KT}{8\pi SJ}\right]^{3/2} Z(3/2)\right] \qquad (2.5.12)$$

where $v = V/l^3$ = number of atoms per elementary cell and is 1, 2, and 4 for simple cubic, body centered cube and face centered cube respectively.

Equation (2.5.12) is called the Bloch $T^{3/2}$ particularly in metals with higher Curie temperature. When we compare with the molecular field theory which predicts an exponential increase in magnetisation we can say there is satisfactory agreement.

The energy of the spin is calculated in the same way from equation (2.5.3)

$$E = E_0 + \frac{3N}{2V}\frac{(KT)^{5/2}}{(8\pi SJ)^{3/2}} Z(5/2) \qquad (2.5.13)$$

From this we obtain the magnetic contribution to the specific heat

$$C_m(T) = \left[\frac{\partial E}{\partial T}\right]_{H=0} = \frac{15NK}{4V}\left[\frac{KT}{8\pi SJ}\right]^{3/2} Z(5/2) \qquad (2.5.14)$$

where $Z(5/2) = 1.341$

CHAPTER THREE

3.0 SPIN INTERACTION ENERGY

3.1 The meaning of exchange interaction

Consider all two particles wave functions that can be constructed as a product of the bonding and anti-bonding wave functions of hydrogen ion H_2^+ to be ψ_+ and ψ_- respectively. The lowest of such states has the wave function given by the equation[Crangle,1977]

$$\psi(r_1,r_2) = \psi_+(r_1)\psi_+(r_2) \qquad (3.1.1)$$

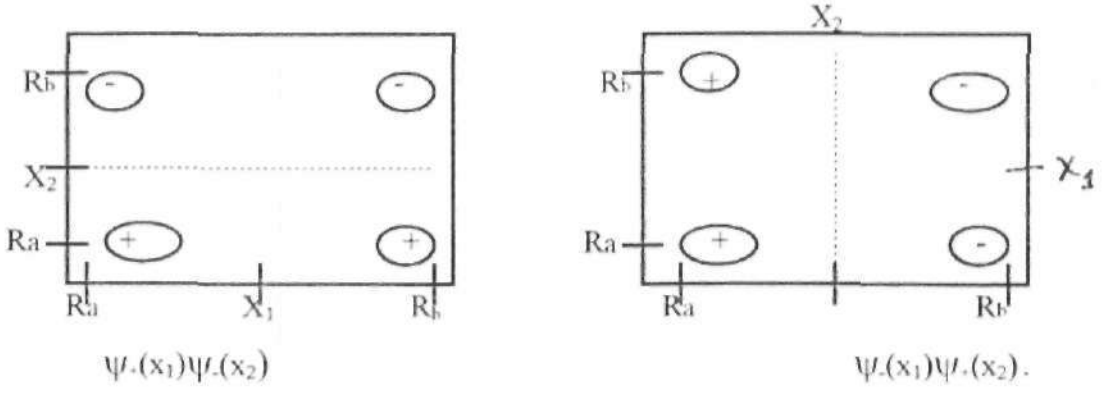
Using the approximate value of ψ_+ that is

$\psi_+(r_1) = \psi_a(r_1) + \psi_b(r_1)$, then equation (3.1.1) can be rewritten as

$$\psi(r_1,r_2) = \psi_a(r_1)\psi_a(r_2)+\psi_b(r_1)\psi_b(r_2)+\psi_a(r_1)\psi_b(r_2)+\psi_b(r_1)\psi_a(r_2) \qquad (3.1.2)$$

Clearly the first two terms are different from the last two terms. In terms of bonding between two atoms A and B, the first term has larger amplitude when both electrons are near the nucleus A and the second term has its largest amplitude when both electrons are near nucleus B. But the last two terms have large amplitude when one electron is near each nucleus. Within the independent particle approximation these states have the same energy. This energy is called the exchange energy[Crangle,1977,and White,1983].

The extension of the above discussion of wave function due to the hydrogen atom to include excited states will enable us to relate the independent particle approximation to the alternative Heitler-London approximation and also make a fuller discussion on the idea of exchange energy[Hall, 1974].



$\psi_-(x_1)\psi_-(x_2)$ (a)

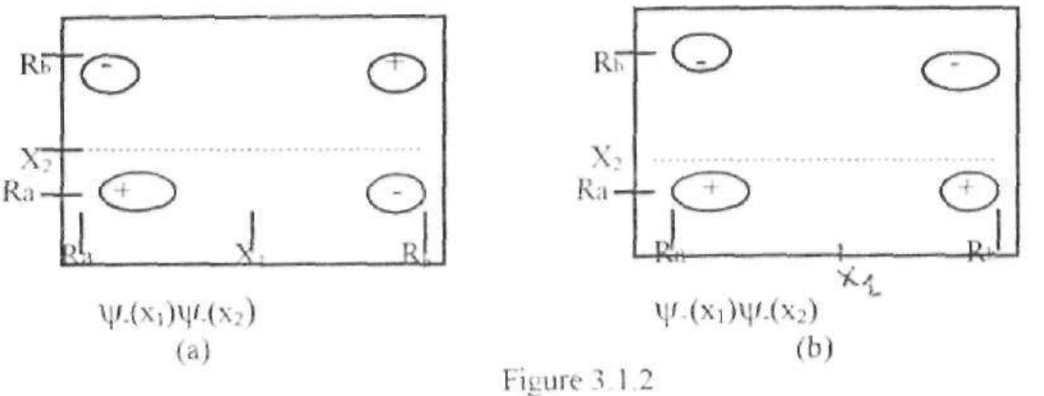
Fig 3.1.1

$\psi_-(x_1)\psi_-(x_2)$. (b)

The above wave function differs only in the levelling of the electrons, as a result they are said to be exchange degenerate . To obtain a physically acceptable wave function from them we have to construct linear combinations that are symmetric and anti-symmetric under the exchange co-ordinates (x_1,x_2), so as to satisfy the equation

$$|\psi(x_1,x_2)|^2 = |\psi(x_2,x_1)|^2 \quad \text{OR} \quad \psi(x_1,x_2) = \pm\psi(x_2,x_1) \tag{3.1.3}$$

We can have the above combinations as in the following Figures[Hall, 1974].



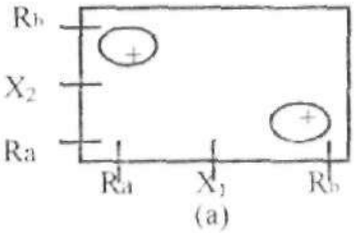
$\psi_+(x_1)\psi_+(x_2)$ (a) $\psi_+(x_1)\psi_+(x_2)$ (b)

Figure 3.1.2

The acceptable representation comes from Heitler-London approximation. If we set

$$\psi_+ = (\psi_a + \psi_b) \qquad \text{and} \qquad \psi_- = (\psi_a - \psi_b)$$

The wave function in Figure 3.1.3 can be expressed alternatively in terms of single atom wave function ψ_a and ψ_b.

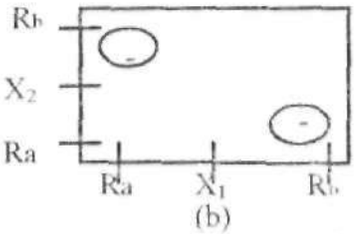


(a)

$\psi_+(x_1)\psi_+(x_2) - \psi_+(x_1)\psi_+(x_2)$ Single state

OR (3.1.4)

$\psi_b(x_1)\psi_a(x_2) + \psi_a(x_1)\psi_b(x_2)$ un-perturbed state



(b)

$\psi_+(x_1)\psi_+(x_2) - \psi_+(x_1)\psi_+(x_2)$ Single state

OR (3.1.5)

$\psi_b(x_1)\psi_a(x_2) - \psi_a(x_1)\psi_b(x_2)$ un-perturbed state

Figure 3.1.3

These figures are the acceptable linear combination of the exchange degenerate states $\psi_a(x_1)\psi_b(x_2)$ and $\psi_b(x_1)\psi_a(x_2)$ and they are good approximation to the lowest two energy states. Accurate energy calculations show that equilibrium separation of the ground state wave function is much closer in Figure 3.1.3 and 3.3.2 than in Figure 3.1.1 [Hall, 1974]. This indicates that the Heitler-London approximation is to be more preferred. But because it can not be extended to more than two electrons, in addition to its conceptual simplicity the independent particle approximation is widely used despite its weaknesses.

The removal of the degeneracy such as the one in Figure 3.1.2 is said to be due to the exchange interaction[White, 1983], a quantum mechanical effect resulting from the requirement that the wave function be symmetric or anti-symmetric under the exchange of particles. The product wave function shown in Figure 3.1.2 both give the same expectation value of the Coulomb interaction $e^2/(4\pi\in_0 |r_1-r_2|)$. But Figures 3.1.1(a) and 3.1.2(a) give quite different expectation value. These two states behave as if there were an energy difference depending on whether the spins are parallel or anti-parallel. Because of the relation between space and spin symmetry, this term is expressed as $-2J\sigma_1\bullet\sigma_2$ in terms of energy, where J = exchange energy term and σ = Pauli spin matrix.

This state always has less Coulomb repulsion. As a result Coulomb repulsion gives a lower energy for parallel spins as in Figure 3.1.1(b) and Figure 3.1.2(a). This is the basis of Hund's rule in atomic spectroscopy.

3.2 Derivation of exchange integral.

Here we wish to evaluate the exchange interaction between two electrons which might be on the same atom, on neighbouring atoms in a crystal or are occupying block states of a crystal lattice. The interaction of two electrons where the un-perturbed state of one, ψ_a, is an eigen state of the Hamiltonian[Crangle,1977 and Hall, 1974]:

$$H_a = -\frac{\hbar^2\nabla^2}{2m} + V_a \qquad (3.2.1)$$

and the un-perturbed state for the other, ψ_b, is an eigen state of the Hamiltonian,

$$H_b = -\frac{\hbar^2}{2m}\nabla^2 + V_b \qquad (3.2.2)$$

is a sufficiently general problem to cover the above cases. The Hamiltonian for the two electrons, including their mutual Coulomb repulsion is therefore

$$H = -\frac{\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2) + \frac{e^2}{4\pi\epsilon_o|r_1 - r_2|} + V(r_1) + V(r_2) \qquad (3.2.3)$$

Where ∇_1 and ∇_2 are del operators with respect to r_1 and r_2 respectively. The total potential V(r) in equation (3.2.3) is $V_a(r) + V_b(r)$ for electrons on neighbouring atom and

$V(r) = V_a(r) = V_b(r)$ for electrons on the same atom or Bloch electrons[Hall,1974].

Let us now use the Hamiltonian of equation (3.2.3) to evaluate the expectation value of energy

$$\langle E\rangle = \frac{\iint \psi^*(r_1,r_2)H\psi(r_1,r_2)d^3r_1 d^3r_2}{\iint \psi^*(r_1,r_2)\psi(r_1,r_2)\,d^3r_1 d^3r_2} \qquad (3.2.4)$$

Using the property of symmetrised (or anti-symmetrised) trial wave function

$$\psi(r_1,r_2) = \psi_a(r_1)\psi_b(r_2) \pm \psi_b(r_1)\,\psi_a(r_2) \qquad (3.2.5)$$

To evaluate equation (3.2.4), we neglect the denominator which is just a normalisation factor.

$$\langle E\rangle = \alpha\iint[\psi_a(r_1)\psi_b(r_2) \pm \psi^*_b(r_1)\,\psi^*_a(r_2)H\psi_a(r_1)\psi_b(r_2) \pm \psi_b(r_1)\psi_a(r_2)]d^3r_1 d^3r_2$$

$$= \alpha\iint[\psi_a^*(r_1)\psi_b^*(r_2)H\psi_a(r_1)\psi_b(r_2)+\psi^*_b(r_1)\psi^*_a(r_2)H\psi_b(r_1)\psi_a(r_2)$$
$$\pm\psi^*_a(r_1)\psi^*_b(r_1)H\psi_b(r_1)\psi_a(r_2) \pm \psi^*_b(r_1)\psi_a(r_1)H\psi_a(r_1)\psi_b(r_2)]d^3r_1 d^3r \qquad (3.2.6)$$

When interchanging the levelling 1 and 2 in the second and fourth terms

$$\langle E\rangle = 2\iint[\psi_a^*(r_1)\psi_b^*(r_2)H\psi_a(r_1)\psi_b(r_2) \pm \psi^*_a(r_1)\psi^*_b(r_1)H\psi_b(r_1)\psi_a(r_2)]d^3r_1 d^3r_2 \qquad (3.2.7)$$

$$\langle E\rangle = 2\iint\psi_a^*(r_1)\psi_b(r_2)H\psi_a(r_1)\psi_b(r_2)\psi d^3r_1 d^3r_2 \pm 2\iint\psi_a^*(r_1)\psi_b(r_2)H\psi_a(r_1)\psi_b(r_2)d^3r_1 d^3r_2$$

We see that it is the second term which changes the sign according to the symmetry of the wave function and it is the exchange energy. It is positive for spin s=0 and negative for spin s=1. For a spin ½ particle

$$\langle E\rangle = \iint\left[\psi_a^*(r_1)\psi_b(r_2)H\psi_a(r_1)\psi_b(r_2) \pm \psi_a(r_1)\psi_b(r_2)H\psi_b(r_1)\psi_a(r_1)\right]d^3r_1d^3r_2$$

$$= E + J_{ab} \qquad (3.2.8)$$

Where,

$$E = \iint\psi_a^*(r_1)\psi_b(r_2)H\psi a(r_1)\psi b(r_2)d^3r_1d^3r_2 \qquad (3.2.9)$$

and

$$J_{ab} = \iint\psi_a(r_1)\psi_b(r_2)H\psi_b(r_1)\psi_a(r_2)d^3r_1d^3r_2 \qquad (3.2.10)$$

is called the exchange integral.

In the first energy approximation we can write equation (3.2.10) as

$$J_{ab} = \iint\psi_a^*(r_1)\psi_b^*(r_2)V\psi_b(r_1)\psi a(r_2)\,dv_1dv_2$$

Since J_{ab} is positive and finite, this means that the triplet always has lower energy than the singlet, which is just Hund's rule. We can also derive the exchange energy density, as follows: remembering that

$$\left(\frac{-\hbar^2}{2m}\nabla^2 + V_a\right)\psi_a = E_a\psi_a$$

and

$$\left(\frac{-\hbar^2}{2m}\nabla^2 + V_b\right)\psi_b = E_b\psi_b \qquad (3.2.11)$$

from equation (3.2.9) we have

$$I = \iint\psi_a^*(r_1)\psi_b^*(r_2)V\left[E_a+E_b+\frac{e^2}{4\pi\epsilon_o|r_1-r_2|}+V(r_1)-V_b(r)+V(r_2)-V_a(r_2)\right]^3\psi_b(r_1)\psi_a(r_2)\,d^3r_1d^3r_2$$

$$= \iint\psi_a^*(r_1)\psi_b^*(r_2)(E_a+E_b)\psi_b(r_1)\psi_a(r_2)d^3r_1d^3r_2$$
$$+ \iint\psi_a^*(r_1)\psi_b^*(r_2)\frac{e^2}{4\pi\epsilon_o|r_1-r_2|}\psi_b(r_1)\psi_a(r_2)\,d^3r_1d^3r_2$$
$$+ \int\psi_b^*(r_2)\psi_a(r_2)d^3r_2\int\left[V(r_1)-V_b(r_1)\right]\psi_a^*(r_1)\psi_b(r_1)d^3r_1$$
$$+ \int\psi_a^*(r_1)\psi_b(r_2)d^3r_1\int\left[V(r_2)-V_a(r_2)\right]\psi_b^*(r_2)\,\psi_a(r_2)d^3r_2 \qquad (3.2.12)$$

If we are considering two electrons on the same atom, ψ_a and ψ_b are eigen state of the potential $V_a(r) = V_b(r) = V(r)$, and therefore the second and the third terms would vanish and only the first term remains. This term has the form of the Coulomb self energy for a so called exchange charge density defined by

$$\psi(r) = \psi_a(r)\psi_b(r) \qquad (3.2.13)$$

for real ψ_a, ψ_b and which shows that exchange density is always positive. It also serve to explain Hund's rule that spins on the same atom tend to align parallel since this corresponds to an anti-symmetric space function [Ruderman at el,1954].

3.3 HEISENBERG HAMILTONIAN IN SECOND QUANTIZATION

Heisenberg Hamiltonian can be derived conveniently using the second quantisation approach[White, 1983]. The Hamiltonian for a system of N electrons localised on N lattice sites is given by

$$H = \sum_{T} \frac{p_i^2}{2m} - \sum_{i,\alpha} \frac{Ze^2}{(r_i - R)} + \frac{1}{2}\sum_{ij} \frac{e^2}{|r_i - r_j|} \qquad (3.3.1)$$

where $\sum_{T} \frac{p_i^2}{2m}$ = Kinetic energy of ion

$-\sum_{i,\alpha} \frac{Ze^2}{|r_i - R|}$ = Potential due to ion-lattice interaction.

and $\frac{1}{2}\sum_{ij} \frac{e^2}{|r_i - r_j|}$ = Electron-Electron interaction

The field operator for the above Hamiltonian can be constructed from a set of Wannier functions.

$$\psi(r) = \sum_{\alpha,n,} Q_n(r-R)a_n(R_\alpha) \qquad (3.3.2)$$

Thus,

$$H = \sum_{KL} \langle K|T|L\rangle a_K^{\dagger} a_L + \frac{1}{2}\sum \langle KL|V|St\rangle a_K^{\dagger} a_l^{\dagger} a_s a_t \qquad (3.3.3)$$

The second term of equation (3.3.3) becomes,

$$\tfrac{1}{2}\sum_{\alpha_1\alpha_2\alpha_3\alpha_4}\langle\alpha_1 n_1\alpha_2 n_2 \mid V \mid \alpha_3 n_3\alpha_4 n_4\rangle a^{+}_{n_1\lambda_3}(R_{\alpha_1})a^{+}_{n_2\lambda_2}(R_{\alpha_2})a_{n_4\lambda_4}(R_{\alpha_4})a_{n_3\lambda_1}(R_{\alpha 3}) \quad (3.3.4)$$

The main contribution to the above equation arises from those terms in which $\alpha_3=\alpha_1$ and $\alpha_4=\alpha_2$ or $\alpha_3=\alpha_2$ and $\alpha_4=\alpha_1$. This is because of the fact that Wannier states are localised within a unit cell.

If we keep only those terms where $n_3=n_1$, and $n_4=n_2$ equation (3.3.4) can be written as

$$\tfrac{1}{2}\sum_{\substack{\alpha,\alpha'\\ n,n'\\ \lambda,\lambda'}}\langle\alpha_i n_j\alpha' n' \mid V \mid \alpha_i n_j\alpha' n'\rangle a^{+}_{n,\lambda}(R_{\alpha'})a_{n',\lambda'}(R_{\alpha'})a_{n',\lambda'}(R_{\alpha'})$$

$$+\langle\alpha_i n_j\alpha' n' \mid V \mid \alpha' n'_i\alpha_n\rangle a^{+}_{n}(R_{\alpha'})a^{+}_{n}(R_{\alpha})a_{n',\lambda'}(R_{\alpha})a_{n',\lambda'}(R_{\alpha'}). \quad (3.3.5)$$

The first term is the direct term while the second term is the exchange term. If we use the Fermion anti commutation relation

$$a^{+}_{n}(R_{\alpha}).a_{n'\lambda'}(R_{\alpha'}) = \delta_{\alpha,\alpha'}\delta_{n,n'}\delta_{\lambda,\lambda'} \quad (3.3.6)$$

The exchange term which is the second term of equation (3.3.5) becomes

$$-\tfrac{1}{2}\sum_{\substack{\alpha,\alpha'\\ n,n'\\ \lambda,\lambda'}} J_{nn'}(R_{\alpha}R_{\alpha'})a^{+}_{n}(R_{\alpha})a_{n}(R_{\alpha})a^{+}_{n',\lambda'}(R_{\alpha'})a_{n',\lambda'}(R_{\alpha'}) \quad (3.3.7)$$

The negative sign is as a result of interchanging of $a_n(R_\alpha)$ and $a^{+}_{n',\lambda'}(R_{\alpha'})$. If we allow only one electron per each orbital we have

$$N_n\uparrow(R_\alpha) + N_n\downarrow(R_\alpha) = 1 \quad (3.3.8)$$

where $N_n\uparrow(R_\alpha) = a^{+}_{n}\downarrow(R_\alpha)a_n(R_\alpha)$ is the number operator associated with the n^{th} orbital with sign at site α. We also have

$$N_n\uparrow(\vec{R_\alpha}) - N_n\downarrow(\vec{R_\alpha}) = \sigma_z(\vec{R_\alpha}) \quad (3.3.9)$$

Combining equation (3.3.8) and (3.3.9) we have

$$N_n\uparrow(\vec{R_\alpha})N_{n'}\uparrow(\vec{R_\alpha}) + N_n\downarrow(\vec{R_\alpha})N_{n'}\downarrow = \tfrac{1}{2}\sigma_z(\vec{R_\alpha})\sigma_z(\vec{R_{\alpha'}}) + \tfrac{1}{2}$$

Also $$a^{+}_{n}(\vec{R_\alpha})a_n\downarrow(\vec{R_\alpha}) = \tfrac{1}{2}\sigma^{+}(\vec{R_\alpha}) \quad (3.3.11)$$

and $a_{n\downarrow}(\overrightarrow{R_\alpha})a_{n\uparrow}(\overrightarrow{R_\alpha}) = \frac{1}{2}\sigma^{-}(\overrightarrow{R_\alpha})$ (3.3.12)

Therefore expanding equation (3.3.7) the exchange becomes

$$-\sum_{\alpha,\alpha'} J_{nn'}(R_\alpha R_{\alpha'})[\frac{1}{4} + \frac{1}{4}\,\sigma(R_\alpha)\bullet\sigma(R_{\alpha'})] \qquad (3.3.13)$$

The interaction can be expressed in terms of total spin as

$$H_{ex} = -\sum_{\alpha,\alpha} J_{nn'}(R_\alpha R_{\alpha'})[\frac{1}{4} + S(R_\alpha)\bullet S(R_{\alpha'})] \qquad (3.3.14)$$

This is the Heisenberg exchange interaction. This is the starting point in theoretical study of Ferromagnetism and anti-ferromagnetism. Expanding equation (3.3.14) we have

$$H_{ex} = -\frac{1}{4}\sum_{\alpha,\alpha} J_{nn'}(R_\alpha R_{\alpha}) - \sum_{\alpha,\alpha} J_{nn'}S(R_\alpha)\bullet S(R_{\alpha'}) \qquad (3.3.15)$$

By redefining our zero energy we can eliminate the constant term and write

$$H_{ex} = -\sum J_{ij}S_i(R_i)\bullet S_j(R_j)] \qquad (3.3.16)$$

3.4 The s-d interaction

Although ferromagnetic metals and alloys of 3d transition elements such as iron, cobalt and nickel are among the best known and useful groups of materials which have been studied extensively both theoretically and experimentally nevertheless, the origin of the ferromagnetism is not yet obvious[Rado Suhl,1966 and Cohen, 1968]. It is clear that the main part of magnetic moments comes from the 3d electrons. Many models have been proposed in order to explain the main mechanism of the alignment of the magnetic moments of the 3d electrons. The first model was based on the Heitler-London localised d-electron model and Heisenberg- type d-d exchange interaction. Another one was proposed by Stoner [Stoner,1938] based on the band model for the 3d electrons. These two models, are completly opposite extreme models, because in the first one the intra atomic d-d Coulomb interaction is assumed to dominate over the interatomic transfer interaction, where as the reverse is the case in the second model in which it was assumed that the band energy is much

greater than the correlation energy[Rado Suhl,1966]. The fact that in the actual 3d electrons, localised and band characteristics are probably mixed nearly equally, is the most difficult obstacle to a satisfactory theoretical understanding of ferromagnetism in 3d metals.

The third model, which considers the problem of configuration mixing was proposed by Zener [Rado Suhl,1966] which differs from the former two in that instead of the d-d interaction, the exchange interaction between 3d electrons and the conduction electrons, which are mainly of 4s character, are most important for the alignment of the 3d magnetic moments. This model is what is called an "S-d interaction model"[Rado Suhl ,1966].

3.5 The Molecular Field Approximation

For an isotropic ferromagnet in an external field H, which is parallel to the Z-axis we have

$$\mathbf{H} = g\mu_B H \sum_{i=1}^{N} S_{iz} - 2\sum_{i>j} J_{ij}(S_i \cdot S_j) \qquad (3.6.1)$$

In the mean field approximation, one of the angular momenta S_j is replaced by the thermal mean $\langle S_j \rangle$, and because of the translational symmetry, $\langle S_j \rangle$ will be independent of the lattice site and anti-parallel to the external field.

Therefore $$\mathbf{H} = g\mu_B (H + B_W) \sum_{i=1}^{N} S_{jz} \qquad (3.6.2)$$

$$B_W = (g\mu_B)^{-1} 2\sum_{j=1}^{N} J_{ij} \langle S_{jz} \rangle \qquad (3.6.3)$$

is called Weiss molecular field.

In this approximation the exchange coupling has the same effect as a magnetic field inside the medium. Because of translational symmetry this is independent of the subscript i.

Since electron spin and magnetic spin are anti parallel to each other, the magnetisation is given by

$$M = -Ng\mu_B \langle S_{jz} \rangle = -B_W \qquad (3.6.4)$$

B_W is called the Weiss constant ($\chi = T_c/C$). A problem of many spins have been reduced to just a problem of one spin.

For a ferromagnetic ion, the susceptibility is given by

$$\chi = \frac{Ng\mu_B JB_J}{H} \quad (\beta g_J \mu_B JH) \tag{3.6.5}$$

where J is the total angular momentum quantum number, $\beta = 1/(K_B T)$

$$B_{J(X)} = \frac{1}{2J}[(2J+1)\mathrm{Coth}\{((2J+1)/2J)x\} - \mathrm{Coth}(x/2J) \tag{3.6.6}$$

is called the Brillouin function. Using equation (3.6.3) and (3.6.5) we have the magnetisation

$$M = Ng\mu_B sB_S(\beta g\mu_B s(H+B_W)) \tag{3.6.7}$$

s = atomic spin quantum number, g= gyro-magnetic factor. If H =0 in the above equation we have spontaneous magnetisation. It vanishes at T_c. near $T=T_c$ the Brillioun function can be expanded as follows:

$$B_S(x) = \frac{(s+1)}{3s}x - \frac{(2s+1)^4 - 1}{(2s)^4}\frac{x^3}{45} + \ldots \tag{3.6.8}$$

So that from equations (3.6.6)and (3.6.8) we have

$$M^2 = 10NK\frac{s(s+1)}{s^2+(s+1)^2}\frac{T^2(T_c-T)}{T_c^2} \tag{3.6.9}$$

True if $T<T_c$, above T_c, M=0.

$$\text{Where } KT_c = \frac{N\mu_B^2 g^2 s(s+1)}{3} \tag{3.6.10}$$

If the exchange is decreasing rapidly with distance then we can restrict our selves to nearest neighbours interaction. Every atom has Z nearest neighbours denoted by J between nearest neighbours. We have according to equations (3.6.2), (3.6.3) and (3.6.10)

$$KT_c = \frac{2ZJs(s+1)}{3} \tag{3.6.11}$$

above Curie point M α H. that is, M= χH.

Using equation (3.6.8) we have

$$X = \frac{C}{T-T_c} \quad ; C = \frac{Ng^2\mu_B^2 s(s+1)}{3K} \tag{3.6.12}$$

In the molecular approximation, the mean energy E = -MH -½ sing equation (3.6.2) and (3.6.4)), ½ mean spin been counted twice. Near Curie point M and energy vary rapidly with temperature. For H= 0 the magnetic contribution to specific heat is

$$C_m(T) = -½\left[\frac{M^2}{T}\right]_{H=0} \tag{3.6.13}$$

above the Curie temperature C_m vanishes. That is C_m =0 if $T>T_c$. Just below Tc we apply the Brillouin function expansion equation (3.6.7) and use equation (3.6.10) to obtain

$$C_m(T) = \frac{NK5s(s+1)}{s^2+(s+1)^2}\ \frac{T^2}{T_c^2}(1+2(1-\frac{T_c}{T}) \tag{3.6.14}$$

Below Curie point specific heat increases as the square of the temperature and drop to zero at $T = T_c$ showing discontinuity:

$$C_m = \frac{NK\ 5s(s+1)}{s^2+(s+1)^2} \tag{3.6.15}$$

The discontinuous beha iour of specific heat indicates a second order phase transition from ferromagnetic to the paramagnetic state. The molecular theory describes only the long range order in the system considered.

Calculation of $J = \frac{3KT_c}{2Z(s^2+1)s}$, from equation (3.6.11)

For Iron T_c = 1093K, Z=8, K=3.86x10^{-6}eV K^{-1}, s=1.1

therefore J= 0.004908 eV K^{-1}

For Nickel T_c=631K, Z=12, K=3.86x10^{-6}eV K^{-1}, s=0.3

Therefore J= 0.00078 eV K^{-1}

For Gadolinium T_c = 289K, Z =12, $K=3.86\times10^{-6}$eV K^{-1}, s=3.6

From which J= 0.00000842 eV K^{-1}

For Tb Tc=218K, Z=12, $K=3.86\times10^{-6}$eV K^{-1}, s=3,

therefore J=0.000008765 eV K^{-1}

For Dy Tc=90K, Z=12, $K=3.86\times10^{-6}$eV K^{-1}, s=2.5,

therefore J= 0.00000496 eV K^{-1}

For Ho, Tc =20, Z=12, $K=3.86\times10^{-6}$eV K^{-1}, s=3,

therefore J= 0.000001608 eV K^{-1}

For Er Tc=20, Z=12, $K=3.86\times10^{-6}$eV K^{-1}, s=1.3,

from which J= 0.000003114 eV K^{-1}

From the result for J the theory doesn't cater for all magnetic substances.

CHAPTER FOUR

4.0 MAGNETISM OF RARE EARTH METALS

4.1 Ruderman-Kittel (Indirect) Interaction

The indirect exchange theory of magnetism in metals is an example in which the effective Heisenberg Hamiltonian can be derived by the second order perturbation theory. This theory which was first proposed in connection with nuclear magnetic resonance by Ruderman and Kittel [Ruderman et al 1954] and independently by Bloembergen and Rowland [Hao Che et al 1992] was based on the fact that beside the localised d or f-electrons the conduction electrons may also contribute to exchange interaction [Mattis, 1981]. The idea was used to study the effect of long range interaction between nuclear spins due to hyperfine coupling with the common sea of conduction electrons. The extension of this analysis to the s-d or s-f interaction permitted the explanation of ferromagnetism in rare earth metals [Vonsovskii 1977]. Since the wave function of the 4f electrons of neighbouring atoms can overlap only very little, a direct exchange interaction is possible in the case of rare-earth metals. But according to the Ruderman-Kittel idea, the conduction electrons are polarised by the direct exchange interaction with the magnetic d or f electrons[Hao Che,et al1992], which means that they are particularly oriented, so that the d or f electrons are coupled in this way. The strength of this interaction decreases gradually with distance, in a manner we are going to calculate [Mattis, 1976].

Let us assume a pair of solute magnetic atoms at distance R_1 and R_2 to be in an ideal non-magnetic metal with s-band Hamiltonian H_O. The magnitudes of the solute spins are mainly fixed at S_1 and S_2 respectively by the internal Hund's rule. But interaction will be governed by the R-K interaction, which we will derive below[Ododo, 1994]. The exchange coupling of the localised electrons is given by the perturbation Hamiltonian as

$$H_{ex} = -J_{cll}\left[S_1 \bullet S_C(R_1) + S_2 \bullet S_C(R_2)\right] \qquad (4.1.1)$$

Where $S_c(R_i)$ is the conduction-band spin operators given by

$$S_p^z = \tfrac{1}{2}(n_{p\uparrow} - n_{p\downarrow}) = (C^*_{p\uparrow}C_{p\uparrow} - C^*_{p\downarrow}C_{p\downarrow})$$

$$S^+_p = S^x_p + iS^y_p = C^*_{p\uparrow}C_{p\downarrow} \text{ and} \qquad (4.1.2)$$

$$S^-_p = S^x_p - iS^y_p = C^*_{p\downarrow}C_{p\uparrow}$$

The occupation number $n_p = C^*_p \bullet C_p$, where C_p and C_p are the Wannier operators.

Substituting these Wannier operators by Bloch operators

$$C_{K,n,m} = \frac{1}{\sqrt{N}}\sum_{i=1}^{N}\exp(-iK\bullet R_i)C_{i,n,m}$$

$$C^*_{K,n,m} = \frac{1}{\sqrt{N}}\sum_{i=1}^{N}\exp(iK\bullet R_i)C^*_{i,n,m}$$

$$\psi_{tk}(r) = \mathrm{Exp}(iK\bullet r)U_{tk}(r) \qquad (4.1.3)$$

Let us introduce new Bloch operators as follows

$$S_c(R_i)^z = \frac{1}{2N}\sum_{K,q}\exp(-iq\bullet R_i)(C_{K,q\uparrow}C_{K\uparrow} - C_{K+q\downarrow}C_{K\downarrow})$$

$$S_c(R_i)^+ = \frac{1}{N}\sum_{K,q}\exp(-iq\bullet R_i)(C^*_{K+q\uparrow}C_{K\downarrow}) \qquad (4.1.4)$$

$$S_c(R_i)^- = \frac{1}{N}\sum_{K,q}\exp(-iq\bullet R_i)(C_{K+q\downarrow}C_{K\uparrow})$$

where $q = K-K'$

Applying these substitution to equation (4.1.1) gives:

$$H_{ex} = -J_{eff}\sum_{i=1}^{2}\{S_c(R_i)^z S_i^z + \tfrac{1}{2}[S_c(R_i)^+ S_i^-]\} \qquad (4.1.5)$$

after using ordinary perturbation theory and the assumption that the conduction electrons are in their ground state, except for the resultant polarisation effect [Mattis.1981]. If we use the notation $|F_g \bullet t\rangle$ to indicate the product state of the Fermi sea with the two solute spins t from 1 to r, we find that the first order correction to the energy vanishes. That is,

$$\delta F^{(1)} = (t \quad |H_{ex}|F,t) = 0 \tag{4.1.6}$$

The conduction band spin operators C^*C create elementary excitation of energy $E(K+q) - E(K)$, in which the matrix elements are unity if $K < K_F$ and $|K+q| > K_F$ and equals zero otherwise. Therefore by using the second order perturbation theory, the second order perturbation gives

$$E_n^{(2)} = -\left[\frac{J_{eff}}{2N}\right]^2 \sum_{\substack{n,K<K_F \\ |K+q|>K_F}} \frac{\langle n|\exp(i\vec{q}\cdot\vec{R}_1)S_1^- + \exp(i\vec{q}\cdot\vec{R}_2)S_2^-|n'\rangle\langle n'|\exp(-i\vec{q}\cdot\vec{R})S_1^+|n\rangle}{E(K+q) - E(K)} \tag{4.1.7}$$

we use $|n\rangle$ to be the ground state and $|n'\rangle$ to the excited state.

Let us make use of the relation,

$$\sum_{n'} |n\rangle\langle n'| = 1, \quad S = S(S+1) \quad \text{and} \quad S_1 \cdot S_2 = S_1 S_2 \cos(q \cdot R_2) \tag{4.1.8}$$

Equation (4.1.7) becomes

$$E_n^{(2)} = -\frac{(J_{eff})^2}{(2N)^2} \sum \frac{\langle n|S_1(S_1+1)+S_2(S_2+1)+S_1S_2\cos(q\cdot R_{12})|n\rangle}{E(K+q) - E(K)} \tag{4.1.9}$$

Equation (4.1.9) can be separated into two, the self-energy

$$\delta E^{(2)} = -K_1 \sum_i S_i(S_i+1) \tag{4.1.10}$$

where $$K_1 = \frac{(J_{eff})^2}{(2N)^2} \sum_{\substack{K \\ |K+q|>K_F}} \frac{1}{E(K+q) - E(K)},$$

and the interaction energy (coupled pair) which is the eigenvalue of the effective Hamiltonian

$$H_{IE} = \sum_{i,j} J(R_{ij})_{IE}\, S_i \cdot S_j \tag{4.1.11}$$

where $$J(R_{ij}) = \frac{(J_{eff})^2}{N^2} \sum_{\substack{K \\ |K+q|>K_F}} \frac{\cos(q\cdot R_{ij})}{E(K+q) - E(K)} \tag{4.1.12}$$

called the indirect exchange coupling. To get an estimate of the above indirect coupling, we use the effective mass approximation $E(K) = \frac{\hbar^2 K^2}{2m^*}$ and $\mu = \frac{\hbar^2 K_F^2}{2m^*}$

Let a_O^3 be the volume of a unit cell, then changing the above summation sign into the integration, we have

$$J(R_{ij}) = J_{eff}^2(a_O/2\pi)^6\int_{E(K)\le\mu} d^3K\int d^3K' \frac{2\mathrm{Cos}(K-K')\bullet R_{ij}}{(h^2/2m)\bullet(K^2+-K'^2)}$$

$$=J_{eff}^2(a_O/2\pi)^6\iint \{\mathrm{Cos}(K\bullet R_{ij}\mathrm{Cos}\theta)\mathrm{Cos}(K'R_{ij}\mathrm{Cos}\theta')+\mathrm{Sin}(KR_{ij}\mathrm{Cos}\theta)\mathrm{Sin}(K'R_{ij}\mathrm{Cos}\theta')\}\bullet$$

$$(2\pi)^2K^2K'^2\mathrm{Sin}\theta d\theta\mathrm{Sin}\theta' d\theta' dKdK' \qquad (4.1.13)$$

Integrating over θ,θ' we have

$$J(R_{ij})_{IE} = J_{eff}^2(a_O/2\pi)^6\bullet(m^*/2h^2)\bullet(4\pi/R_{ij})^2\int_0^{K_F} KdK\int_{-\infty}^{\infty} K'dK'\frac{\mathrm{Sin}R_{ij}}{K'^2-K^2}\,\mathrm{Sin}K'R_{ij}dKdK' \qquad (4.1.14)$$

We use the contour technique to evaluate the integral K' with K' from $-\infty$ to $+\infty$. To avoid the singularities we form semicircles at the points $K' = \pm K$ to get the equivalent of

$$I(\sigma) = \int_{-\infty}^{\infty}\frac{x\mathrm{Sin}x dx}{x^2-\sigma^2} \qquad (4.1.15)$$

which is from the quantum mechanical analysis of scattering:

$$= \int_{-\infty}^{\infty} K'\frac{\mathrm{Sin}(K'R_{ij})}{K'^2-K^2}\,dK' \qquad (4.1.16)$$

Multiplying by $(R_{ij})^2$ we have

$$= \int_{-\infty}^{\infty}\frac{K'R_{ij}\mathrm{Sin}(K'R_{ij})d(K'R_{ij})}{(K'R_{ij})^2-(Kr_{ij})^2} \qquad (4.1.17)$$

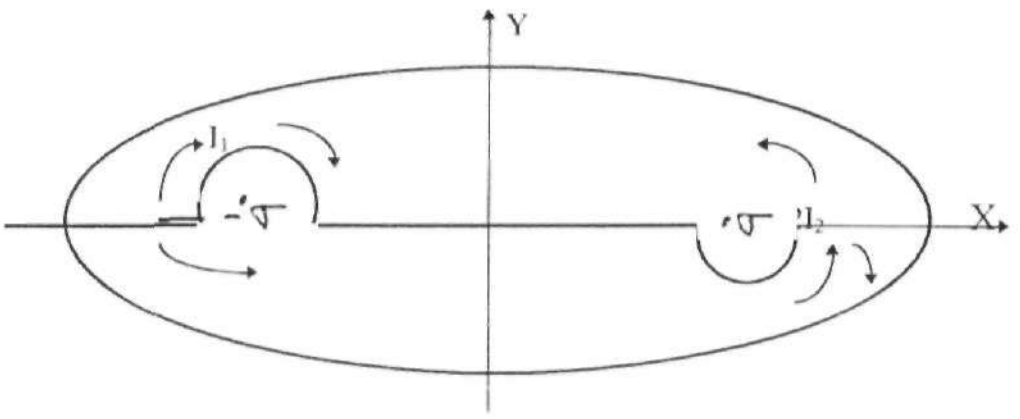
To evaluate the above integral we use, $\mathrm{Sin}(z) = \frac{e^{iz}-e^{-iz}}{2i}$

equation (4.1.15) can be written in the complex plane as

$$I = I_1 + I_2 \qquad (4.1.18)$$

with, $I_1 = \frac{1}{2i}\int_{-\infty}^{\infty}\frac{ze^{iz}}{z^2-\sigma^2}dz$, $I_2 = \frac{1}{2i}\int_{-\infty}^{\infty}\frac{ze^{-iz}}{z^2-\sigma^2}dz$

The contour of I_1 is completed by forming an infinite semicircle in the upper half plane and the reverse is the case for I_2[Arfken,1985].



Fig

Figure 4.1.1

The poles are at $z = +\sigma$ and $z = -\sigma$ on the contour of integration.

$Z = \sigma$ and $z = -\sigma$, $I_1 = \frac{e^{i\sigma}}{2}$ and $I_1 = \frac{e^{-i\sigma}}{2}$, $I_2 = \frac{e^{-i\sigma}}{2}$ and $I_2 = \frac{e^{i\sigma}}{2}$ (4.1.19)

The residue theorem leads to

$$I_1 = \pi_i(1/2i)\frac{e^{-i\sigma}}{2} + \pi_i(1/2i)\frac{e^{i\sigma}}{2} = 2\pi_i(1/2i)\frac{e^{i\sigma}}{2} \quad (4.1.20)$$

For the clockwise singularity and

$$I_2 = -\pi_i(-1/2i)\frac{e^{i\sigma}}{2} + \pi_i(-1/2i)\frac{e^{-i\sigma}}{2} = -2\pi_i(-1/2i)\frac{e^{i\sigma}}{2} \quad (4.1.21)$$

For the anti-clockwise.

Adding the above equations we have

$$I(\sigma) = I_1 + I_2 = \pi/2(e^{i\sigma}+e^{i\sigma}) = \pi\mathrm{Cosh}(i\sigma).$$

This implies that,

$$I(\sigma) = \pi Cos\sigma \tag{4.1.22}$$

Hence the integral is

$$\int_{-\infty}^{\infty} \frac{K'Sin(K'R_{ij})dK'}{K'^2-K^2} = \int_{-\infty}^{\infty} \frac{K'R_{ij}Sin(k'R_{ij})d(K'R_{ij})}{(K'R_{ij})^2 - (KR_{ij})^2} = \pi Cos(K'R_{ij}) \tag{4.1.22}$$

Putting this in equation (4.1.14) we have

$$J(R_{ij})_{IE} = J_{eff}^2(a_O/2\pi)^6(m^*/2h^2)(4\pi/R_{ij})^2\int_0^{K_F}\pi KSin(KR_{ij})Cos(KR_{ij})dk \tag{4.1.23}$$

Using the trigonometry relation $Sin\theta Cos\theta = \frac{1}{2}Sin2\theta$, we obtain the expression

$$\int_0^{K_F} KSin(KR_{ij})Cos(KR_{ij})dK = \tfrac{1}{2}\pi\int_0^{K_F} KSin(2KR_{ij})dK$$

Multiplying top and bottom by $(2R_{ij})^2$, we have

$$\tfrac{1}{2}\pi\int_0^{K_F} \frac{2KR_{ij}Sin(2KR_{ij})d(2KR_{ij})}{(2R_{ij})^2} \tag{4.1.24}$$

Integrating by parts, that is. $\int vdu = uv - \int udv$, by letting $u=Sin(2KR_{ij})$, and $du=d(Sin2KR_{ij})$

and $dv = d(2KR_{ij})$ and $v = 2KR_{ij}$

gives

$$\tfrac{1}{2}\pi\int_0^{K_F} \frac{2KR_{ij}Sin(2KR_{ij})d(2KR_{ij})}{(2kr_{ij})^2} = \frac{\pi}{2(2Rij)^2}\left[\frac{2K_FR_iSin(2K_FR_{ij})}{2K_FR_{ij}} - 2K_FR_{ij}Cos(2K_FR_{ij})\right]$$

$$= \frac{\pi}{2(2R_{ij})^2}\left(Sin(2K_FR_{ij}) - 2K_FR_{ij}Cos(2K_FR_{ij})\right)$$

putting this in the expression for $J(R_{ij})_{IE}$ above we finally obtain

$$J(R_{ij})_{IE} = (J_{eff}/N)^2 \bullet \frac{K_Fa_O}{(2/(2\pi))}\left[\frac{Sin(2K_FR_{ij}) - 2K_FR_{ij}Cos(2K_FR_{ij})}{(2K_FR_{ij})}\right] \tag{4.1.25}$$

This is the Ruderman-Kittel original formula.[Mattis, 1967] On comparing with the Heisenberg direct exchange we can see that it decreases less rapidly with the increasing distance of the atom. This makes it reasonable to think that indirect exchange may play a decisive role in the case of metals like rare-earth. The interaction is a decreasing oscillatory function of the separation between the localised spin(R_{ij}) and can take the correct sign to give rise to ferromagnetism[Mattis,1981 and Ododo,1994]. To account for the finite electronic mean free path, a factor $e^{-(R_j/\lambda)}$ is introduced, where λ is the mean free path and a_0 is the volume of a unit cell. Therefore we write

$$J(R_{ij})_{IE} = (J_{eff}/\mu)^2\left[\frac{K_f a_0^{1/2}}{2\pi^3}\right]^6\left[\frac{\mathrm{Sin}(2K_F R_{ij})-2K_F R_{ij}\mathrm{Cos}(2K_F R_{ij})}{(2K_j R_{ij})^4}\right]e^{-Rij/\lambda} \qquad (4.1.26)$$

The above Ruderman-Kittel interaction is valid under the following conditions (a) $(J_{NI}^{III}/\mu N) << 1$, (b) There must be no level crossing and (c) The elementary excitations must be particle like. So to plot the curve of the above exchange interaction we let K_F go to zero and replace the sum by integral and use the above conditions. Neglecting the constant terms for simplicity we write

$$E(K) = \sum \frac{a^3[\mathrm{Sin}(2K_F R_{ij})-2K_j R_{ij}\mathrm{Cos}(2K_j R_{ij})]}{5(2K_F R_{ij})R_{ij}^3}\exp(-R_{ij}/\lambda) \qquad (4.1.27)$$

Let $x_j = 2K_F R_{ij}$ therefore,

$$E(K) = \sum \frac{a^3[\mathrm{Sin}x_j - x_j\mathrm{Cos}x_j\exp](-R_{ij}/\lambda)(1-\mathrm{Cos}x_i(K\bullet R_{ij}))}{5x_j R^3_{ij}} \qquad (4.1.28)$$

This is the magnon energy.

Thus we can write the Weiss mean field θ which is proportional to the exchange as

$$\theta = \sum_{R_{ij}\neq 0} \frac{(a^3\mathrm{Sin}x_j - x_j\mathrm{Cos}x_j)}{5x_j R_{ij}^3}\exp(-R_{ij}/\lambda) \qquad (4.1.29)$$

where a = separation of the nearest-neighbours atoms.

The graph of θ as a function of K_F for the various lattice points is provided in appendix III

CHAPTER FIVE

5.00 RESULTS AND DISCUSSION

5.1 Ordered Magnetic Materials:

As mentioned in chapter one, at low temperature paramagnetic materials have been divided into two different classes. The basis for the distinction is provided by magnetic order as described in section 1.2. A Ferro-magnet has a spontaneous magnetic moment. That is, the alignment of spontaneous atomic or molecular moments with respect to the crystallographic axes. A spontaneous moment suggests that electron spins and magnetic moments are arranged in a regular manner.

Generally, the f-shell radii of the rare earth atoms are so small that even nearest neighbouring atoms do not have significant direct overlap and the interaction is assumed to be the Rudermann - Kittel indirect exchange (derived in section 4.1) As a result, the rare-earth series (Gadolinium rare-earth series) and the ordered alloys containing transition elements which have their magnetic atoms sufficiently far apart for the d-shell overlaps to be unimportant are also described by this theory and are refered to as the ordered magnetic materials. This leads to the consideration of the Hamiltonian.

$$H_E = - \sum_{i \neq j} J_{ij} S_i \cdot S_j \qquad (5.1.1)$$

and the calculation of eigen-states and eigen values for the case in which the spin occupy points on a regular lattice. It is assumed to be on the Bravais lattices and on one of the three principal cubic lattices.

The ground states is obtained by first constructing the product wave function

$$\Psi = \Pi\varnothing_I \qquad (5.1.2)$$

$\varnothing_i$ = Unspecified but normalised states of the spin S_i

The variational energy in this configuration is

$$E = (\Psi|H_{II}|\Psi) - \sum J_{ij} (\varnothing_i|S_i|\varnothing_i) (\varnothing_j|S_j|\varnothing_j) \qquad (5.1.3)$$

where $(\varnothing_i|S_i|\varnothing_i)^2 \leq S_i^2$ --- (5.1.4)

Assuming all N_I magnetic atoms to belong to the same species, so that $S_i = S$.

A spherical model can be used to find the lowest energy using the trial wave function of equation (5.1.2). This consists of relaxing the inequality equation (5.1.4) requiring only the weaker constraint.

$$\sum_i (\varnothing_i|S_i|\varnothing_i)^2 \leq N_I S^2 \qquad (5.1.5)$$

The value of equation (5.1.3) is lowest under the rigorous constraint equation (5.1.4). The energy E in equation (5.1.3). is calculated by Fourier transforms, letting

$$(\varnothing_i|S_i|\varnothing_i) = \sum e^{ik.Ri} S_k \qquad (5.1.6)$$

substituting in equation (5.1.3) we have

$$E = C \sum_k J(k)|S_k|^2 \qquad (5.1.7)$$

where $J(k) = \frac{1}{2}N_I \sum_{ij} J_{ij} e^{ik.Rij}$ ... (5.1.8)

when we substitute equation (5.1.6) into equation (5.1.5). we have

$$\sum_k |S_k|^2 \leq S^2 \qquad (5.1.9)$$

Let us define q_o to be the wave vector for which $J(k_o)$ attain its largest values

then $E(q_o) = - N_l J(q_o) S^2$ (5.1.10).

This is the lowest energy subject to the weak constraint.

If we now choose the wave function $\varnothing_i$ such that

$$(\varnothing_i|S_i|\varnothing_i) = S\,(\cos q_o, R_i, \sin q_o, R_i 0) \ldots\ldots\ldots \quad (5.1.11)$$

Inserting this in equation (5.1.3). lead to equation (5.1.10) and being an upper and as well as lower bound to the ground state energy. when all spins are parallel and the ground state is ferromagnetic, either wise the ground state is anti-ferromagnetic. This shows that numerical calculation is required to obtain J(k), and to determine q_o in the case of the long-ranged Rudermann-Kittel interaction unlike the case of short-ranged Heisenberg interaction in which the proof holds also. The numerical calculation of J(o) is particularly interesting, because it is proportional to the Weiss Mean Field (WMF) which is also proportional to the paramagnetic Curie temperature θ. Negative θ necessarily precludes Ferro-magnetism ; a positive θ is a likely indication of Ferro-magnetism; but, it is still possible for $q \neq o$ to be the ground state solution. This makes it necessary to study the spin - wave spectrum.

$$\hbar\omega(k) = 2s\,\{J(o) - J(k)\} \ldots\ldots\ldots\ldots \quad (5.1.12)$$

to determine that all $\hbar w(k)$ are positive, if the ferromagnetism; state is to be stable. This is the necessary but not sufficient condition for Ferro-magnetism. The $\hbar w(k)$ for the R-K interaction in the limit $K_F a \rightarrow o$ where the lattice sums can be replaced by integrals is

$$E(k) = \sum a^3 \; \sin x_i - x_i \cos x_i \; e^{-Ri\,|\lambda} \frac{(1 - \cos k \bullet R_i)}{5\, x_i \cos R_i^3} S_i \quad (5.1.13)$$

which is the magnon energy with the constant vector eliminated, for tabular convenience.

5.2 Evaluation of Weiss Mean Field:

The Weiss Mean Field (WMF) which is proportional to the paramagnetic curie temperature θ can be evaluated from equation (4.1.29) was solved over all allowed valuesof the lattice points R_i. Given the equation the basic differences in the WMF for the three lattices, simple cubic, body centred and face centred is in the calculation of the radius wave vector R which is dependent on the integer lattice point l, m and n. The values of equation (4.1.29) are tabulated with the sum over allowed lattice points $R_i = \sqrt{(l^2 + m^2 + n^2)}$ except $R_i = 0$. For the simple cubic SC all integer value of l, m, and n are allowed, this condition was taken care by a program written for the calculation of WMF for SC.

The condition on the wave vector R_i for the body centered cubic (BCC) is that l, m, n must be all even or all odds. The computer programme for the calculation of WM. for BCC also takes care of it. The condition on l, m, and n for the face centred cubic (FCC)is that l + m + n must be equal to even integer, and this is used in the computation of the WMF for FCC. All these WMF are evaluated with the value of a = 1 and $\lambda = 3$.

The rare earth metals have the hexagonal close packed crystal structure. For HCP, a proof for the condition is given in appendix I. It is shown that the structure factor for HCP is given by $1 + e^{i\,\pi n}$, n = 1, 2.....6 where n is an integer. The computer programme for evaluating the WMF of HCP was also written.

The result of the computation are presented for SC, BCC, FCC and HCP in table I through table IV respectively. A plot of WMF against $K_F a$ is also presented from figure (I) through figure (IV) respectively. The plots are found to be in good agreement with corresponding ones obtained in literature.

5.3 Evaluation of Energy:

The energy spectrum is calculated using the formula

$$E(k) = \sum \frac{(a^3 \mathrm{Sin}x_i - x_i \mathrm{Cos}x_i)\exp(-R_{ij}/\lambda)\,(1-\mathrm{Cos}k\bullet Ri)}{5x_i R_i^3} \qquad (5.3.1)$$

On the basis of Rudermann Kittel exchange interaction . the calculation of E(k) is the same as for W.M.F except for an additional superposed term $(1-\cos l_i\pi q_x \cos m_i\pi q_i \cos n_i\pi q_i)$. Here q represents the direction and x is taken from 0 to 1.00 in interval of 0.5. For the HCP lattice the energy has been calculated for the three directions [100], [110] and [111]. and presented in appendix II.

5.3 Conclusions:-

The Pauli exclusion principle keeps electron with parallel spins apart and so reduces their Coulombic repulsion. The difference between parallel spin configuration and the anti-parallel one is the exchange energy. This is however favourable to Ferromagnetism only if it is positive. In order for exchange to occur, the paths of the interacting electrons must inevitably and in extrically overlap. The Heisenberge nearest neighbours exchange mechanism, assume that electrons in well localised magnetic d or f shells interact with one another in an extremely distinct way from those in Bloch states that account for the metallic properties. Because of the fact that in rare earth metals the magnetic shells are well localised (~0.3Å) that, the overlap between atoms must be negligibly small, and hence Heisenberg approximation may not hold. The observed magnetism in such a case involves conduction electrons, which are capable of sustaining correlation over several inter-atomic distance. As a

result we give a general review of exchange interaction in chapter two and three of this project the result we displayed at the end of chapter three show that it is not very much applicable to the rare earth metals.

In an attempt to understand the Rudermann Kittel exchange interaction a suitable expression of it was derived in chapter four. The analysis of the derived relation was carried out by computer programming in BASIC language. The result is displayed in graphical forms. In addition we present a proof for the condition used in evaluating WMF and Magnon energy for hexagonal closed packed structure (HCP) in appendix I. It is the principal object of the magnetic theory in metal to explain precisely how the electronic interactions modify the Fermi Sea and perturb the ground state energy. It is only in rare earth metals such conditions were satisfied, because the Hund's rule energy which is responsible for the existence of atomic magnetic moment must be larger than the bonding energy as measured by the Fermi energy. The key to magnetic behaviour must be the existence of degenerate bands.

The calculation of the WMF which is proportional to the magnetic Curie temperature was carried out. The plot gives the characteristics of the indirect RKKY exchange interaction between local magnetic moment situated in a bulk pure metals, that is, oscillation which falls with distance. This oscillation are caused by a singularity in dielectric functions to the sharp Fermi surface. It is shown through plotting of all the lattices SC, BCC, FCC and HCP (appendix III) that WMF goes through zero and then encounter an anti-ferromagnetic region (below zero) and rises again to ferromagnetic region and then a new anti ferromagnetic region is encountered and so on. The plots also show spins stable regions $\hbar\omega(k) > 0$ which are the peaks of the positive part of the plots.

Tables of values of the functions WMF for all the four lattices are also presented in appendix II. The result is obtained by summing over twenty thousand (20,000) lattice points. Tables of values for the Magnon energy E(k) for the SC along [100] direction as a test case was produced. It was found to agree with the one obtained in the literature.

As an extension we performed calculation for HCP along [100], [110] and [111] also summing about twenty thousand lattice points. We give a plot of WMF and E(k) against K_F for HCP along the two directions for the first time. Choosing different K_F at x = 0.5, the shape of the energy plot against K_F closely followed that of WMF against K_F as expected

The table of values for the Magnon energy E(k) were also produced for SC along [100] and HCP along the three directions. These results were produced using a computer programme written in BASIC language. Like that of the literature the numerical values show no dependence on the mean free path (λ) . As a result it serves only as an ultimate cut-off and convergence factor. Small value of K_F were considered, because it was found that they agree extremely well with the analytic calculation given in equation (4.1.29). In addition to this R -K interaction is long range there by giving us another reason for using small K_F.

We conclude that the criteria of the molecular field theory are met at lowest temperature where spin wave theory is applicable. The indirect theory is applicable mainly for the description of the magnetic properties of the rare earth metals and alloys.

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APPENDIX I

PROOF OF GEOMETRICAL STRUCTURE FACTOR (S) FOR HCP LATTICE

The geometrical structure factor which is defined as an integral over a single cell with r = 0 at a corner is given by

$$S = \sum_j \int dVn_j (r - r_j) \exp(- iG\bullet r) \qquad A1.1$$

$$= \sum_j \exp(- iG\bullet r_j) \int dVn_j (\rho) \exp(- iG\bullet\rho) \qquad A1.2$$

Where $\rho \equiv r - r_j$

Let us define the atomic form factor as

$$F_j = \int dVn_j (\rho) \exp(- iG\bullet\rho) \qquad A1.3$$

Therefore the structure factor becomes

$$S_G = \sum_j f_j \exp(- iG\bullet r_j) \qquad A1.4$$

We know that $r_j = x_j a + y_j b + z_j c$

$a = ax$, $b = ay$ and $c = a = az$

and $G = hA + KB + Lc$

where $A = \dfrac{b \times c}{a_\bullet b \times c} = \dfrac{2\pi x}{a}$

where $B = \dfrac{2\pi y}{a}$ and $C = \dfrac{2\pi z}{a}$

$$r_j\bullet G = (ax_j x + ay_j y + az_j z)\bullet(ha + KB + lC)$$

$$= a[x_j x + y_j y + z_j z] \bullet [(2\pi/a) hx + (2\pi/a) ky + l(2\pi/a) lz]$$

$$= a(x_j x + y_j y + z_j z) \bullet (2\pi/a) (h x + ky + l z)$$

$$= 2\pi (x_j h + y_j k + z_j z)$$

Therefore $S(hkl) = \sum_j f_j \exp\{-2\pi i (x_j h + y_j k + z_j l)\}$

The HCP lattice has a basis of two atoms one at (0,0,0) and the other at ($^2/_3$, $^1/_3$, $^1/_2$).

If (x, y, z) = (0,0,0).

$$\mathbf{S}(hkl) = \sum_j f_j \exp[-2\pi i (x_j h + y_j k + z_j z)]$$

$$= \sum_j f_j \exp[-2\pi i (0)]$$

$$= \sum_j f_j \exp(-0)$$

$$= \sum_j f_j$$

If (x, y, z) = ($^2/_3$, $^1/_3$, $^1/_2$)

$$\mathbf{S}(h\ k\ l) = \sum_j f_j \exp(-2\pi i (^2/_3 h + {}^1/_3 k + {}^1/_2 l)$$

Therefore

$$\mathbf{S}(h\ k\ l) = \sum_j f_j (1 + \exp(-2\pi i (^2/_3 h + {}^1/_3 k + {}^1/_2 l))$$

$$= \sum_j f_j (1 + \exp[(-2\pi i/3)(2h + k + {}^2/_3 l)])$$

$$= \sum_j f_j (1 + \exp(-2\pi i (4h + 2k + 3l))]$$

$$= \sum_j f_j (1 + \exp[(-\pi i/3)(4h + 2k + 3l)]$$

$$= \sum_j f_j (1 + \exp(-i\pi/3)(n_1 + n_2 + n_3)$$

$$= \sum_j f_j (1 + \exp(-i\pi n/3)$$

Where $n = n_1 + n_2 + n_3$ = 1 to 6

APPENDIX II

TABLE 1

Table of values for Fermi Wave Vector (K_F) and Weiss Mean Field (WMF) for Simple Cube (SC)

K_F	WMF	K_F	WMF	K_F	WMF
0.2	0.657670	4.2	-0.068782	8.2	0.953939
0.4	1.173988	4.4	0.307433	8.4	0.273255
0.6	1.364605	4.6	0.751768	8.6	-0.416248
0.8	1.380036	4.8	0.851365	8.8	-0.927635
1.0	1.283537	5.0	0.705851	9.0	-1.174488
1.2	1.106791	5.2	0.482528	9.2	-1.238093
1.4	0.874263	5.4	0.321263	9.4	-0.941734
1.6	0.605503	5.6	0.164182	9.6	-0.465233
1.8	0.314276	5.8	-0.162529	9.8	-0.118522
2.0	0.014555	6.0	-0.553566	10.0	0.274437
2.2	-0.273063	6.2	-0.861814	10.2	0.509818
2.4	-0.521537	6.4	-1.027098	10.4	0.656963
2.6	-0.698191	6.6	-1.114952	10.6	0.680306
2.8	-0.756957	6.8	-0.984768	10.8	0.443387
3.0	-0.624929	7.0	-0.433920	11.0	0.150305
3.2	-0.286647	7.2	0.262046	11.2	-0.054425
3.4	-0.065933	7.4	0.689377	11.4	0.006963
3.6	-0.052365	7.6	1.080679	11.6	0.198748
3.8	-0.125572	7.8	1.488870	11.8	0.560927
4.0	-0.171101	8.0	1.433696	12.0	0.573387

TABLE 2

Table of values for Fermi Wave Vector (K_F) and Weiss Mean Field (WMF) for Body-Centered Cube (BCC)

K_F	WMF	K_F	WMF	K_F	WMF
0.2	0.155065	4.2	0.129310	8.2	0.236014
0.4	0.257010	4.4	0.099123	8.4	0.145105
0.8	0.209990	4.6	0.058131	8.6	0.046451
0.6	0.261497	4.8	-0.002421	8.8	-0.049708
1.0	0.124128	5.0	0.006779	9.0	-0.170892
1.2	0.019652	5.2	-0.023813	9.2	-0.188725
1.4	-0.086411	5.4	-0.115770	9.4	-0.133529
1.6	-0.173096	5.6	-0.162351	9.6	-0.008753
1.8	-0.212338	5.8	-0.071835	9.8	0.160170
2.0	-0.161688	6.0	0.129578	10.0	0.203330
2.2	0.026220	6.2	0.150211	10.2	0.169223
2.4	0.212674	6.4	0.061535	10.4	0.069227
2.6	0.221681	6.6	0.007788	10.6	-0.068328
2.8	0.122484	6.8	0.024461	10.8	-0.192047
3.0	0.002058	7.0	-0.005135	11.0	-0.260648
3.2	-0.082302	7.2	-0.059666	11.2	-0.149135
3.4	-0.160190	7.4	-0.116112	11.4	0.008276
3.6	-0.192494	7.6	-0.142262	11.6	0.226023
3.8	-0.078488	7.8	-0.078667	11.8	0.320370
4.0	0.099415	8.0	0.107712	12.0	0.180927

TABLE 3

Table of values for Fermi Wave Vector (K_F) and Weiss Mean Field (WMF) for Face Centered Cube (FCC)

K_F	WMF	K_F	WMF	K_F	WMF
.2	.3212031	4.2	-.4313488	8.2	.2870869
.4	.5569148	4.4	-.4492455	8.4	.1198755
.6	.6160486	4.6	-.3532538	8.6	-.2429658
.8	.5759279	4.8	-.3003783	8.8	-.5761693
1	.4712465	5	-.1665856	9.0	-.697327
1.2	.3218977	5.2	.204795	9.2	-.498573
1.4	.1456133	5.4	.6055417	9.4	6.103512E-02
1.6	-4.059115E-02	5.6	.6985201	9.6	.4393087
1.8	-.2198995	5.8	.4838939	9.8	.4801241
2	-.3714475	6.0	.1152875	10.0	.4304839
2.2	-.4648011	6.2	-.257234	10.2	.3284279
2.4	-.4547971	6.4	-.5339067	10.4	.2535037
2.6	-.275875	6.6	-.6688029	10.6	.0384053
2.8	7.444859E-02	6.8	-.5039193	10.8	-.33213
3	.3615426	7.0	-5.833649E-02	11.0	-.6053454
3.2	.544604	7.2	.2566204	11.2	-.5670599
3.4	.5343988	7.4	.2919264	11.4	-.3035429
3.6	.3380976	7.6	.2700899	11.6	-.1196287
3.8	5.308064E-02	7.8	.3142115	11.8	.1687061
4	-.2328979	8.0	.2920686	12.0	.5134934

TABLE 4

Table of Values for Fermi Wave Vector (K_F) and Weiss Mean Field (WMF) for Hexagonal Close Pack (HCP)

K_F	WMF	K_F	WMF	K_F	WMF
0.20	2.414924	4.20	-3.330130	8.20	5.399817
0.40	6.508274	4.40	-3.947657	8.40	5.090089
0.60	8.303256	4.60	-4.390126	8.60	4.456105
0.80	8.420805	4.80	-4.679273	8.80	3.565324
1.00	8.641567	5.00	-4.590907	9.00	2.662486
1.20	8.828674	5.20	-3.833371	9.20	2.065511
1.40	8.535687	5.40	-2.482063	9.40	1.823649
1.60	7.989722	5.60	-1.050415	9.60	1.540106
1.80	7.433560	5.80	-0.113483	9.80	0.778873
2.00	6.843958	6.00	0.124692	10.00	-0.430319
2.20	6.098358	6.20	-0.085541	10.20	-1.894212
2.40	5.194232	6.40	-0.425683	10.40	-3.379894
2.60	4.274196	6.60	-0.799110	10.60	-4.522349
2.80	3.381393	6.80	-1.137137	10.80	-5.306012
3.00	2.407541	7.00	-1.293122	11.00	-5.915111
3.20	1.346186	7.20	-1.127953	11.20	-6.321898
3.40	0.321252	7.40	-0.335370	11.40	-6.650683
3.60	-0.630814	7.60	1.387549	11.60	-6.884316
3.80	-1.571440	7.80	3.554899	11.80	-6.335541
4.00	-2.505328	8.00	5.041082	12.00	-4.445089

Table 5

K_F, WMF, AND ENERGY (E) ALONG X: (1 0 0) FOR SIMPLE CUBIC LATTICE (SC). (E IS IN ARBITRY UNITS)

kf= 0.20 wmf= .6576705

x	E
0.00	0.000000
0.05	0.047566
0.10	0.214066
0.15	0.518779
0.20	0.938244
0.25	1.435920
0.30	1.983471
0.35	2.564093
0.40	3.167456
0.45	3.786592
0.50	4.417114
0.55	5.056262
0.60	5.701788
0.65	6.352122
0.70	7.006321
0.75	7.663433
0.80	8.322752
0.85	8.983488
0.90	9.645357
0.95	10.307920

kf = 0.60 wmf= 1.364605

x	E
0.00	0.000000
0.05	0.010705
0.10	0.056487
0.15	0.165373
0.20	0.364648
0.25	0.681159
0.30	1.143750
0.35	1.775702
0.40	2.580025
0.45	3.535547
0.50	4.609354
0.55	5.771602
0.60	7.000123
0.65	8.278890
0.70	9.595407
0.75	10.940560
0.80	12.307046
0.85	13.689212
0.90	15.081838
0.95	16.480459

kf = 1.00 wmf= 1.283537

x	E
0.00	0.000000
0.05	0.005529
0.10	0.026134
0.15	0.069832
0.20	0.145951
0.25	0.265350
0.30	0.438619
0.35	0.676720
0.40	0.992516
0.45	1.399894
0.50	1.913365
0.55	2.548925
0.60	3.320370
0.65	4.230171
0.70	5.264133
0.75	6.397902
0.80	7.606241
0.85	8.868306
0.90	10.166505
0.95	11.485505

kf = 0.4 wmf= 1.173988

x	E
0.00	0.000000
0.05	0.023178
0.10	0.115901
0.15	0.325049
0.20	0.692868
0.25	1.240667
0.30	1.956344
0.35	2.803908
0.40	3.745783
0.45	4.755101
0.50	5.813615
0.55	6.907976
0.60	8.029244
0.65	9.171065
0.70	10.328526
0.75	11.497710
0.80	12.675857
0.85	13.860763
0.90	15.049877
0.95	16.241510

kf=0.80 wmf= 1.380036

x	E
0.00	0.000000
0.05	0.007047
0.10	0.035795
0.15	0.101477
0.20	0.219475
0.25	0.406280
0.30	0.680040
0.35	1.059850
0.40	1.566052
0.45	2.218887
0.50	3.030029
0.55	3.992556
0.60	5.082516
0.65	6.271364
0.70	7.535321
0.75	8.855962
0.80	10.218429
0.85	11.611030
0.90	13.023944
0.95	14.448785

kf = 1.20 wmf= 1.106791

x	E
0.00	0.000000
0.05	0.003266
0.10	0.015870
0.15	0.043516
0.20	0.092400
0.25	0.169061
0.30	0.279952
0.35	0.431926
0.40	0.632507
0.45	0.889536
0.50	1.211450
0.55	1.607848
0.60	2.089134
0.65	2.666488
0.70	3.351348
0.75	4.149972
0.80	5.055767
0.85	6.048401
0.90	7.101437
0.95	8.189620

kf =1.40 wmf =.8742626

x	E
0.00	0.000000
0.05	0.001270
0.10	0.007428
0.15	0.023267
0.20	0.052896
0.25	0.099707
0.30	0.167686
0.35	0.261154
0.40	0.384001
0.45	0.540303
0.50	0.734725
0.55	0.971797
0.60	1.256081
0.65	1.592977
0.70	1.988197
0.75	2.447369
0.80	2.976466
0.85	3.579117
0.90	4.249976
0.95	4.969445
1.00	5.706405

kf = 2.20 wmf =-.2730632

x	E
0.00	0.000000
0.05	-0.001441
0.10	-0.006623
0.15	-0.017385
0.20	-0.036360
0.25	-0.067058
0.30	-0.113301
0.35	-0.179742
0.40	-0.272467
0.45	-0.398820
0.50	-0.567699
0.55	-0.789456
0.60	-1.072321
0.65	-1.417542
0.70	-1.818786
0.75	-2.266339
0.80	-2.750455
0.85	-3.262136
0.90	-3.792948
0.95	-4.335110
1.00	-4.881001

kf = 3.00 wmf = -.6249289

x	E
0.00	0.000000
0.05	-0.006825
0.10	-0.030859
0.15	-0.075488
0.20	-0.138435
0.25	-0.215182
0.30	-0.301089
0.35	-0.391931
0.40	-0.484060
0.45	-0.574550
0.50	-0.661122
0.55	-0.742129
0.60	-0.816493
0.65	-0.883616
0.70	-0.943325
0.75	-0.995965
0.80	-1.042305
0.85	-1.083452
0.90	-1.120767
0.95	-1.155853
1.00	-1.190193

kf = 1.80 wmf= .3142766

x	E
0.00	0.000000
0.05	0.000847
0.10	0.003410
0.15	0.007638
0.20	0.013907
0.25	0.022970
0.30	0.034942
0.35	0.049480
0.40	0.066237
0.45	0.084295
0.50	0.101890
0.55	0.116787
0.60	0.125881
0.65	0.124500
0.70	0.106589
0.75	0.064510
0.80	-0.010976
0.85	-0.126831
0.90	-0.281356
0.95	-0.462633
1.00	-0.653179

kf = 2.60 wmf=-.6981915

x	E
0.00	0.000000
0.05	-0.002923
0.10	-0.015376
0.15	-0.045039
0.20	-0.100012
0.25	-0.189314
0.30	-0.322883
0.35	-0.508350
0.40	-0.747069
0.45	-1.034329
0.50	-1.363010
0.55	-1.726290
0.60	-2.118157
0.65	-2.533441
0.70	-2.967765
0.75	-3.417362
0.80	-3.878786
0.85	-4.349031
0.90	-4.825349
0.95	-5.305209
1.00	-5.786047

kf = 3.40 wmf= -0.06593253

x	E
0.00	0.000000
0.05	0.005531
0.10	0.027337
0.15	0.074078
0.20	0.149712
0.25	0.253032
0.30	0.380092
0.35	0.526883
0.40	0.690303
0.45	0.868156
0.50	1.059123
0.55	1.262707
0.60	1.478908
0.65	1.707969
0.70	1.950383
0.75	2.206571
0.80	2.476546
0.85	2.759353
0.90	3.052909
0.95	3.353678
1.00	3.656987

kf = 3.80 wmf=-.1255717

x	E
0.00	0.000000
0.05	-0.000771
0.10	-0.003756
0.15	-0.010125
0.20	-0.020875
0.25	-0.037105
0.30	-0.059753
0.35	-0.089333
0.40	-0.127507
0.45	-0.179917
0.50	-0.256830
0.55	-0.370109
0.60	-0.529188
0.65	-0.738973
0.70	-0.999584
0.75	-1.306999
0.80	-1.654204
0.85	-2.032597
0.90	-2.433180
0.95	-2.847007
1.00	-3.265140

kf = 4.60 wmf= .7517684

x	E
0.00	0.000000
0.05	0.010746
0.10	0.051662
0.15	0.136718
0.20	0.272870
0.25	0.460656
0.30	0.696639
0.35	0.976222
0.40	1.295288
0.45	1.650284
0.50	2.038211
0.55	2.456576
0.60	2.903641
0.65	3.377928
0.70	3.878335
0.75	4.404049
0.80	4.954513
0.85	5.528934
0.90	6.125456
0.95	6.738308
1.00	7.357409

kf = 5.40 wmf= .3212619

x	E
0.00	0.000000
0.05	-0.000665
0.10	-0.003117
0.15	-0.007676
0.20	-0.013300
0.25	-0.017832
0.30	-0.018932
0.35	-0.014714
0.40	-0.003687
0.45	0.015445
0.50	0.044059
0.55	0.084716
0.60	0.142939
0.65	0.228026
0.70	0.351521
0.75	0.523778
0.80	0.750037
0.85	1.027555
0.90	1.345618
0.95	1.688588
1.00	2.039784

kf = 4.20 wmf=-0.06878227

x	E
0.00	0.000000
0.05	-0.007374
0.10	-0.036684
0.15	-0.101362
0.20	-0.211607
0.25	-0.372086
0.30	-0.581283
0.35	-0.832917
0.40	-1.118044
0.45	-1.426735
0.50	-1.749079
0.55	-2.075443
0.60	-2.396267
0.65	-2.703283
0.70	-2.991829
0.75	-3.261869
0.80	-3.516811
0.85	-3.760743
0.90	-3.997226
0.95	-4.229331
1.00	-4.460045

kf =5.00 wmf= .7058513

x	E
0.00	0.000000
0.05	0.001843
0.10	0.009587
0.15	0.027930
0.20	0.061866
0.25	0.116525
0.30	0.197612
0.35	0.311788
0.40	0.466075
0.45	0.665784
0.50	0.911750
0.55	1.198949
0.60	1.517882
0.65	1.857778
0.70	2.208552
0.75	2.561321
0.80	2.908674
0.85	3.246524
0.90	3.575249
0.95	3.898222
1.00	4.219339

kf = 5.80 wmf=-.1625319

x	E
0.00	0.000000
0.05	0.001522
0.10	0.007768
0.15	0.022077
0.20	0.047448
0.25	0.086470
0.30	0.142075
0.35	0.218032
0.40	0.317836
0.45	0.442546
0.50	0.589738
0.55	0.754290
0.60	0.929782
0.65	1.109216
0.70	1.285128
0.75	1.449481
0.80	1.593866
0.85	1.711241
0.90	1.799561
0.95	1.864996
1.00	1.921772

kf = 6.20 wmf =-.8618163

x	E
0.00	0.000000
0.05	-0.004194
0.10	-0.019649
0.15	-0.050750
0.20	-0.100072
0.25	-0.170040
0.30	-0.263730
0.35	-0.384763
0.40	-0.537229
0.45	-0.725979
0.50	-0.956741
0.55	-1.234498
0.60	-1.559868
0.65	-1.926102
0.70	-2.320232
0.75	-2.728071
0.80	-3.139400
0.85	-3.549224
0.90	-3.956294
0.95	-4.361235
1.00	-4.765430

kf =7.00 wmf = -.433908

x	E
0.00	0.000000
0.05	-0.004551
0.10	-0.021324
0.15	-0.054993
0.20	-0.108095
0.25	-0.182836
0.30	-0.281718
0.35	-0.407156
0.40	-0.561910
0.45	-0.750522
0.50	-0.979547
0.55	-1.255244
0.60	-1.580433
0.65	-1.952995
0.70	-2.367133
0.75	-2.815728
0.80	-3.291932
0.85	-3.789417
0.90	-4.301754
0.95	-4.822642
1.00	-5.346222

kf = 7.80 wmf = 1.488875

x	E
0.00	0.000000
0.05	0.014535
0.10	0.069557
0.15	0.183989
0.20	0.370212
0.25	0.636819
0.30	0.990718
0.35	1.437888
0.40	1.984216
0.45	2.636112
0.50	3.399987
0.55	4.278503
0.60	5.267558
0.65	6.356162
0.70	7.531157
0.75	8.779774
0.80	10.089991
0.85	11.450548
0.90	12.849890
0.95	14.274664
1.00	15.708250

kf = 6.60 wmf = -1.114954

x	E
0.00	0.000000
0.05	-0.005784
0.10	-0.028575
0.15	-0.079822
0.20	-0.173214
0.25	-0.324944
0.30	-0.550144
0.35	-0.858056
0.40	-1.250370
0.45	-1.723873
0.50	-2.274191
0.55	-2.897450
0.60	-3.590121
0.65	-4.348739
0.70	-5.170190
0.75	-6.051611
0.80	-6.989588
0.85	-7.979101
0.90	-9.011708
0.95	-10.073489
1.00	-11.145902

kf = 7.40 wmf = .6893841

x	E
0.00	0.000000
0.05	0.000905
0.10	0.004479
0.15	0.013028
0.20	0.030643
0.25	0.063222
0.30	0.116408
0.35	0.193558
0.40	0.296002
0.45	0.424644
0.50	0.580523
0.55	0.764418
0.60	0.976973
0.65	1.218816
0.70	1.489655
0.75	1.787049
0.80	2.106739
0.85	2.443665
0.90	2.792515
0.95	3.148125
1.00	3.505863

kf = 8.20 wmf = .9539289

x	E
0.00	0.000000
0.05	0.004907
0.10	0.025001
0.15	0.071240
0.20	0.154764
0.25	0.286950
0.30	0.479675
0.35	0.744053
0.40	1.087693
0.45	1.512806
0.50	2.017021
0.55	2.596198
0.60	3.247126
0.65	3.968092
0.70	4.758725
0.75	5.619262
0.80	6.548587
0.85	7.541172
0.90	8.583679
0.95	9.657080
1.00	10.740545

kf = 8.60 wmf =-.4162544

x	E
0.00	0.000000
0.05	-0.004361
0.10	-0.022279
0.15	-0.063367
0.20	-0.136295
0.25	-0.247659
0.30	-0.401579
0.35	-0.599490
0.40	-0.840551
0.45	-1.123017
0.50	-1.444824
0.55	-1.802640
0.60	-2.191266
0.65	-2.605752
0.70	-3.044823
0.75	-3.512835
0.80	-4.017998
0.85	-4.567583
0.90	-5.161658
0.95	-5.789186
1.00	-6.429257

kf = 9.40 wmf = -.9417254

x	E
0.00	0.000000
0.05	-0.005389
0.10	-0.026227
0.15	-0.070718
0.20	-0.145307
0.25	-0.256228
0.30	-0.410184
0.35	-0.612027
0.40	-0.861719
0.45	-1.155017
0.50	-1.487823
0.55	-1.859768
0.60	-2.274227
0.65	-2.736271
0.70	-3.249962
0.75	-3.815636
0.80	-4.428355
0.85	-5.078886
0.90	-5.756244
0.95	-6.449576
1.00	-7.148273

kf = 10.20 wmf = .5098242

x	E
0.00	0.000000
0.05	0.001760
0.10	0.009569
0.15	0.029204
0.20	0.067143
0.25	0.129185
0.30	0.219922
0.35	0.343633
0.40	0.505521
0.45	0.711594
0.50	0.967180
0.55	1.276002
0.60	1.640463
0.65	2.061630
0.70	2.537475
0.75	3.060583
0.80	3.618659
0.85	4.197865
0.90	4.786609
0.95	5.377967
1.00	5.969596

kf = 9.00 wmf = -1.174489

x	E
0.00	0.000000
0.05	-0.003809
0.10	-0.020007
0.15	-0.060240
0.20	-0.140424
0.25	-0.279201
0.30	-0.494653
0.35	-0.802143
0.40	-1.213778
0.45	-1.738084
0.50	-2.379970
0.55	-3.141524
0.60	-4.022146
0.65	-5.016376
0.70	-6.112565
0.75	-7.293858
0.80	-8.541792
0.85	-9.838743
0.90	%-11.167973
0.95	%-12.514797
1.00	%-13.867281

kf = 9.80 wmf = -.1185165

x	E
0.00	0.000000
0.05	-0.002892
0.10	-0.011214
0.15	-0.020272
0.20	-0.019231
0.25	0.004421
0.30	0.060277
0.35	0.152315
0.40	0.279111
0.45	0.437092
0.50	0.624679
0.55	0.843984
0.60	1.099245
0.65	1.394767
0.70	1.734004
0.75	2.118896
0.80	2.548237
0.85	3.016501
0.90	3.514284
0.95	4.030129
1.00	4.552066

kf = 10.60 wmf = .6803023

x	E
0.00	0.000000
0.05	0.007853
0.10	0.037547
0.15	0.098587
0.20	0.195064
0.25	0.327123
0.30	0.494102
0.35	0.696758
0.40	0.936193
0.45	1.210409
0.50	1.512336
0.55	1.831527
0.60	2.157845
0.65	2.484612
0.70	2.808461
0.75	3.127179
0.80	3.437153
0.85	3.733855
0.90	4.014702
0.95	4.282381
1.00	4.544823

kf = 11.00 wmf = .1502967

x	E
0.00	0.000000
0.05	-0.001669
0.10	-0.008797
0.15	-0.026367
0.20	-0.060313
0.25	-0.115604
0.30	-0.193888
0.35	-0.293203
0.40	-0.410793
0.45	-0.547086
0.50	-0.707228
0.55	-0.897956
0.60	-1.121943
0.65	-1.374809
0.70	-1.647540
0.75	-1.931781
0.80	-2.222946
0.85	-2.519399
0.90	-2.820239
0.95	-3.124139
1.00	-3.429046

kf = 11.40
wmf = 6.966759E-03

x	E
0.00	0.000000
0.05	-0.001793
0.10	-0.011141
0.15	-0.038563
0.20	-0.098184
0.25	-0.203763
0.30	-0.364148
0.35	-0.580480
0.40	-0.846412
0.45	-1.150715
0.50	-1.480082
0.55	-1.820799
0.60	-2.159934
0.65	-2.486943
0.70	-2.795680
0.75	-3.084917
0.80	-3.357095
0.85	-3.614635
0.90	-3.859421
0.95	-4.094310
1.00	-4.325402

kf = 11.80 wmf = .5609405

x	E
0.00	0.000000
0.05	0.010978
0.10	0.052430
0.15	0.138270
0.20	0.277411
0.25	0.476450
0.30	0.740966
0.35	1.074247
0.40	1.475314
0.45	1.938767
0.50	2.456470
0.55	3.019457
0.60	3.618597
0.65	4.243838
0.70	4.884379
0.75	5.531093
0.80	6.179909
0.85	6.832832
0.90	7.493899
0.95	8.163710
1.00	8.837408

TABLE 6

K_F, WMF, AND ENERGY (E) ALONG X: (1 0 0),(110) AND (111) DIRECTION FOR HEXAGONAL CLOSE PACK LATTICE (HCP). (E IS ARBITRARY UNITS)

K_F =0.20 WMF = 2.414924

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	0.228890	0.432342	0.613382
0.10	0.808557	1.303650	1.614871
0.15	1.483312	1.933951	2.113382
0.20	1.999832	2.176807	2.271769
0.25	2.242076	2.268035	2.340428
0.30	2.265126	2.332479	2.375702
0.35	2.218587	2.364297	2.397529
0.40	2.226464	2.382581	2.411338
0.45	2.312205	2.402229	2.421162
0.50	2.413009	2.411695	2.427763
0.55	2.455607	2.416997	2.432535
0.60	2.424164	2.425337	2.435687
0.65	2.367576	2.428832	2.438088
0.70	2.349176	2.430128	2.439814
0.75	2.389318	2.434416	2.441257
0.80	2.451272	2.435737	2.442255
0.85	2.479256	2.435355	2.443015
0.90	2.451030	2.437805	2.443403
0.95	2.397066	2.438136	2.443648
1.00	2.370601	2.436758	2.443665

K_F = 0.60 WMF = 8.303256

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	0.274060	0.548578	0.821701
0.10	1.059665	2.085940	3.010870
0.15	2.244577	4.131424	5.406085
0.20	3.644035	5.914279	6.889619
0.25	5.029541	6.992337	7.569213
0.30	6.189531	7.526374	7.922512
0.35	6.999162	7.838213	8.132046
0.40	7.459655	8.049792	8.264585
0.45	7.679208	8.183976	8.352519
0.50	7.802605	8.278611	8.412916
0.55	7.932493	8.349385	8.455562
0.60	8.089710	8.396585	8.486251
0.65	8.232371	8.432759	8.508630
0.70	8.312945	8.461275	8.525133
0.75	8.325158	8.479443	8.537331
0.80	8.308980	8.493731	8.546222
0.85	8.314782	8.505180	8.552527
0.90	8.360385	8.510573	8.556761
0.95	8.418893	8.514348	8.559173
1.00	8.445352	8.516864	8.559951

KF = 0.40 WMF = 6.508274

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	0.453663	0.871275	1.255709
0.10	1.637665	2.808435	3.647463
0.15	3.118141	4.562881	5.258008
0.20	4.433172	5.542906	5.914679
0.25	5.309907	5.962194	6.194531
0.30	5.744107	6 .74926	6.346827
0.35	5.917003	6.313241	6.436850
0.40	6.030380	6.399569	6.494250
0.45	6.180311	6.457796	6.532143
0.50	6.342000	6.500519	6.558460
0.55	6.445720	6.529640	6.577075
0.60	6.463897	6.550828	6.590676
0.65	6.437679	6.567301	6.600555
0.70	6.433619	6.578881	6.607864
0.75	6.481410	6.587344	6.613169
0.80	6.551641	6.593884	6.617059
0.85	6.589990	6.598291	6.619785
0.90	6.571640	6 .31127	6.621710
0.95	6.524347	6.602891	6.622836
1.00	6.500164	6.603472	6.623197

KF = 0.80 WMF = 8.420805

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	0.060537	0.133397	0.217737
0.10	0.301970	0.750780	1.299463
0.15	0.852171	2.127779	3.455776
0.20	1.790888	4.023448	5.665035
0.25	3.055891	5.768326	7.017606
0.30	4.441801	6.913343	7.698267
0.35	5.694341	7.538036	8.090850
0.40	6.634606	7.918142	8.335298
0.45	7.231340	8.183552	8.496729
0.50	7.579422	8.359237	8.606918
0.55	7.812866	8.481785	8.684548
0.60	8.018754	8.575813	8.740051
0.65	8.208695	8.641440	8.780528
0.70	8.352524	8.688536	8.810220
0.75	8.431581	8.726588	8.832179
0.80	8.465182	8.752226	8.848147
0.85	8.492592	8.769107	8.859610
0.90	8.536557	8.782913	8.867105
0.95	8.584527	8.789698	8.871508
1.00	8.605680	8.790462	8.872905

K_F = 1.00 WMF = 8.641567

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	0.057095	0.111088	0.163086
0.10	0.242357	0.463252	0.705102
0.15	0.593770	1.208442	2.013747
0.20	1.159313	2.549096	4.153641
0.25	1.970821	4.329947	6.176545
0.30	3.012305	5.998277	7.402402
0.35	4.200062	7.140522	8.066556
0.40	5.392926	7.802873	8.473755
0.45	6.436649	8.221091	8.736108
0.50	7.223325	8.516876	8.914428
0.55	7.733172	8.720543	9.038755
0.60	8.031969	8.864483	9.127985
0.65	8.225219	8.972816	9.192590
0.70	8.397162	9.051224	9.240092
0.75	8.573683	9.107359	9.274815
0.80	8.728649	9.149462	9.300156
0.85	8.824044	9.179008	9.318154
0.90	8.850288	9.197480	9.330211
0.95	8.836437	9.208669	9.337119
1.00	8.825187	9.212730	9.339466

K_F = 1.40 WMF = 8.535687

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	0.045190	0.092935	0.142971
0.10	0.176527	0.379780	0.596551
0.15	0.385383	0.834466	1.267617
0.20	0.668607	1.410051	2.118466
0.25	1.038017	2.189540	3.522071
0.30	1.522086	3.350920	5.422469
0.35	2.155182	4.851672	7.022282
0.40	2.956266	6.319837	7.989606
0.45	3.906591	7.404129	8.578382
0.50	4.939609	8.084538	8.967872
0.55	5.952633	8.535295	9.233656
0.60	6.838652	8.862931	9.421606
0.65	7.524660	9.093137	9.556342
0.70	7.996402	9.256898	9.654305
0.75	8.295969	9.380198	9.725702
0.80	8.493322	9.466882	9.777553
0.85	8.647625	9.525971	9.814218
0.90	8.781477	9.567573	9.838932
0.95	8.880828	9.590239	9.852958
1.00	8.918196	9.596066	9.857599

K_F = 1.20 WMF = 8.828674

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	0.079017	0.155155	0.228150
0.10	0.295773	0.555934	0.776353
0.15	0.610089	1.117224	1.561460
0.20	1.005461	1.925002	2.961944
0.25	1.515290	3.171950	4.995522
0.30	2.203824	4.791814	6.798256
0.35	3.110492	6.349503	7.886068
0.40	4.198105	7.462309	8.515168
0.45	5.346009	8.137754	8.919362
0.50	6.397914	8.578877	9.188087
0.55	7.234242	8.895612	9.374877
0.60	7.821217	9.116125	9.506851
0.65	8.207324	9.274470	9.602486
0.70	8.475472	9.393200	9.672128
0.75	8.688992	9.477658	9.723488
0.80	8.866975	9.538516	9.760743
0.85	8.998708	9.582740	9.787274
0.90	9.074982	9.610470	9.804781
0.95	9.105766	9.626499	9.814891
1.00	9.112422	9.632509	9.818079

K_F = 1.60 WMF = 7.989722

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	0.018903	0.038264	0.058337
0.10	0.084703	0.178055	0.288919
0.15	0.216177	0.472648	0.797095
0.20	0.424737	0.933591	1.513824
0.25	0.706285	1.523026	2.417786
0.30	1.051681	2.290153	3.838121
0.35	1.467525	3.383528	5.622629
0.40	1.986305	4.780987	7.046851
0.45	2.650904	6.160266	7.912624
0.50	3.478825	7.199639	8.461707
0.55	4.430867	7.868333	8.831737
0.60	5.410267	8.315681	9.088573
0.65	6.298163	8.640946	9.272055
0.70	7.005599	8.871821	9.404556
0.75	7.507843	9.034811	9.501211
0.80	7.841124	9.154213	9.570992
0.85	8.066055	9.237460	9.620413
0.90	8.226398	9.290208	9.653138
0.95	8.331587	9.321173	9.671946
1.00	8.369313	9.332007	9.678030

K_F = 1.80 WMF = 7.43356

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	0.016647	0.032618	0.047836
0.10	0.072891	0.138642	0.196183
0.15	0.181911	0.348597	0.511228
0.20	0.351577	0.700218	1.093936
0.25	0.576757	1.185915	1.852663
0.30	0.844009	1.764567	2.783623
0.35	1.146566	2.483210	4.189849
0.40	1.498465	3.484853	5.845469
0.45	1.935295	4.769223	7.106929
0.50	2.497536	6.057133	7.882079
0.55	3.204290	7.045981	8.389924
0.60	4.032784	7.692719	8.736914
0.65	4.916440	8.129523	8.981270
0.70	5.763779	8.446424	9.156587
0.75	6.488812	8.669795	9.283379
0.80	7.038340	8.826252	9.374808
0.85	7.403282	8.936996	9.439198
0.90	7.612046	9.008479	9.482168
0.95	7.710460	9.048638	9.506624
1.00	7.738047	9.062244	9.514615

K_F = 2.20 WMF = 6.098358

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	0.020661	0.041398	0.062234
0.10	0.075881	0.153207	0.232707
0.15	0.151980	0.310501	0.476042
0.20	0.242152	0.499262	0.759354
0.25	0.354729	0.740166	1.144527
0.30	0.507676	1.083102	1.740034
0.35	0.713292	1.540649	2.466541
0.40	0.966455	2.068602	3.388802
0.45	1.247842	2.687300	4.720394
0.50	1.541615	3.527026	6.107281
0.55	1.853974	4.618249	7.083665
0.60	2.216692	5.739996	7.702184
0.65	2.669679	6.623457	8.124809
0.70	3.232472	7.209673	8.419090
0.75	3.883348	7.601023	8.629223
0.80	4.559945	7.878742	8.778576
0.85	5.180314	8.067080	8.883365
0.90	5.670070	8.185594	8.952201
0.95	5.979437	8.253829	8.991521
1.00	6.084354	8.276917	9.004154

K_F = 2.00 WMF = 6.843958

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	0.023103	0.046168	0.069191
0.10	0.088113	0.174506	0.258213
0.15	0.186807	0.364093	0.523913
0.20	0.316248	0.618695	0.902559
0.25	0.482745	0.976456	1.501301
0.30	0.695790	1.444695	2.246196
0.35	0.957624	1.987833	3.171801
0.40	1.260002	2.648288	4.540822
0.45	1.594383	3.565569	6.057642
0.50	1.968722	4.751570	7.166675
0.55	2.414708	5.957085	7.858679
0.60	2.973438	6.897446	8.323946
0.65	3.663419	7.518381	8.645611
0.70	4.452375	7.936729	8.874301
0.75	5.254781	8.239070	9.038190
0.80	5.963108	8.448739	9.155781
0.85	6.495234	8.590088	9.238246
0.90	6.827850	8.685527	9.293090
0.95	6.992794	8.738285	9.324462
1.00	7.039931	8.753643	9.334673

K_F = 2.40 WMF = 5.194232

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	0.006254	0.012797	0.019596
0.10	0.028579	0.061222	0.096814
0.15	0.074071	0.163431	0.264396
0.20	0.146202	0.320639	0.519917
0.25	0.241474	0.516171	0.819164
0.30	0.353738	0.756970	1.215648
0.35	0.482330	1.087846	1.807473
0.40	0.635717	1.523445	2.515081
0.45	0.825774	2.018475	3.432119
0.50	1.056863	2.581448	4.716610
0.55	1.320258	3.333606	5.975245
0.60	1.601368	4.322290	6.835038
0.65	1.896298	5.356730	7.389538
0.70	2.223353	6.179080	7.771610
0.75	2.615605	6.722748	8.037691
0.80	3.093339	7.081120	8.226154
0.85	3.632130	7.327729	8.356774
0.90	4.150527	7.484042	8.443281
0.95	4.531702	7.569945	8.492450
1.00	4.672008	7.598349	8.508504

K_F = 2.60 WMF = 4.274196

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	0.001053	0.002247	0.003609
0.10	0.010867	0.022954	0.037174
0.15	0.043007	0.088501	0.140734
0.20	0.104628	0.214375	0.338246
0.25	0.188668	0.391294	0.615876
0.30	0.279242	0.588171	0.922518
0.35	0.366021	0.799036	1.315045
0.40	0.454749	1.075430	1.880525
0.45	0.563751	1.453833	2.548885
0.50	0.708434	1.897041	3.445698
0.55	0.887075	2.400319	4.667523
0.60	1.081290	3.071502	5.796854
0.65	1.272511	3.965003	6.549740
0.70	1.461050	4.914262	7.043970
0.75	1.669808	5.675331	7.385767
0.80	1.925564	6.172438	7.622776
0.85	2.229074	6.488285	7.786503
0.90	2.536753	6.695054	7.893163
0.95	2.771622	6.807615	7.953842
1.00	2.859702	6.840513	7.973221

K_F = 3.00 WMF = 2.407541

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	0.008998	0.018013	0.027030
0.10	0.030144	0.060874	0.091411
0.15	0.051433	0.106733	0.160872
0.20	0.066181	0.144062	0.223525
0.25	0.079666	0.184401	0.306438
0.30	0.104354	0.257918	0.459147
0.35	0.147581	0.381757	0.685494
0.40	0.202857	0.532549	0.937638
0.45	0.253259	0.684187	1.287027
0.50	0.284576	0.866426	1.788877
0.55	0.296293	1.126264	2.393413
0.60	0.299195	1.450467	3.257224
0.65	0.299761	1.822205	4.341300
0.70	0.284454	2.319095	5.232496
0.75	0.220006	3.008352	5.806169
0.80	0.074826	3.768346	6.188377
0.85	-0.150956	4.375159	6.444118
0.90	-0.409222	4.741947	6.608890
0.95	-0.617287	4.931363	6.701589
1.00	-0.696994	4.993217	6.731353

K_F = 2.80 WMF = 3.381393

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	0.009553	0.018702	0.027451
0.10	0.034787	0.065114	0.091309
0.15	0.068642	0.125691	0.173647
0.20	0.107040	0.203429	0.293640
0.25	0.152592	0.313641	0.485222
0.30	0.211616	0.460746	0.743331
0.35	0.286871	0.625190	1.021635
0.40	0.372754	0.798649	1.390521
0.45	0.458014	1.026117	1.923912
0.50	0.534487	1.352341	2.557395
0.55	0.604403	1.748792	3.435454
0.60	0.679071	2.196662	4.588676
0.65	0.768532	2.787615	5.594146
0.70	0.869765	3.584903	6.251866
0.75	0.963654	4.443560	6.688881
0.80	1.024922	5.132394	6.988700
0.85	1.039176	5.572624	7.192577
0.90	1.014689	5.833441	7.325590
0.95	0.979302	5.980702	7.400599
1.00	0.963253	6.029763	7.424948

K_F = 3.20 WMF = 1.346186

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	-0.002616	-0.004716	-0.006307
0.10	-0.007750	-0.009754	-0.006236
0.15	-0.009752	-0.003269	0.018464
0.20	-0.005389	0.013787	0.055290
0.25	0.002503	0.035211	0.095177
0.30	0.006384	0.060971	0.159651
0.35	-0.000449	0.105137	0.291611
0.40	-0.018669	0.184082	0.487346
0.45	-0.042843	0.282982	0.704314
0.50	-0.067599	0.373363	1.024106
0.55	-0.096306	0.478636	1.484135
0.60	-0.145904	0.651444	2.053095
0.65	-0.243298	0.889075	2.891779
0.70	-0.413734	1.175830	3.896400
0.75	-0.666519	1.579349	4.678719
0.80	-0.985284	2.160952	5.175642
0.85	-1.327744	2.814007	5.502331
0.90	-1.635311	3.328447	5.708186
0.95	-1.848896	3.600472	5.823056
1.00	-1.925105	3.675324	5.859658

K_F = 3.40 w mf = .3212522

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	-0.005796	-0.011759	-0.017863
0.10	-0.018591	-0.038635	-0.059181
0.15	-0.029264	-0.060255	-0.088116
0.20	-0.033822	-0.063163	-0.079913
0.25	-0.038923	-0.057685	-0.053364
0.30	-0.057757	-0.066138	-0.034869
0.35	-0.099648	-0.096969	-0.009558
0.40	-0.163089	-0.132810	0.076469
0.45	-0.239676	-0.144820	0.222655
0.50	-0.326877	-0.128888	0.392527
0.55	-0.438869	-0.107274	0.673836
0.60	-0.604317	-0.071764	1.087975
0.65	-0.849520	0.020963	1.625206
0.70	-1.177393	0.173901	2.435251
0.75	-1.557506	0.368023	3.352417
0.80	-1.935523	0.662390	4.026585
0.85	-2.256527	1.121570	4.445881
0.90	-2.486599	1.643170	4.709911
0.95	-2.618653	2.022311	4.854438
1.00	-2.660734	2.151749	4.901353

K_F = 3.80 WMF = - 1.57144

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	-0.000848	-0.001411	-0.001702
0.10	-0.008578	-0.014024	-0.016862
0.15	-0.034078	-0.058650	-0.076610
0.20	-0.084219	-0.148334	-0.198965
0.25	-0.156258	-0.270336	-0.350659
0.30	-0.242310	-0.401616	-0.488278
0.35	-0.341061	-0.533683	-0.609987
0.40	-0.466774	-0.676003	-0.731116
0.45	-0.646549	-0.846158	-0.833037
0.50	-0.905243	-1.049073	-0.859240
0.55	-1.247347	-1.265844	-0.821564
0.60	-1.648284	-1.484252	-0.737752
0.65	-2.061714	-1.713304	-0.518988
0.70	-2.438516	-1.937465	-0.178169
0.75	-2.745490	-2.115499	0.318226
0.80	-2.973270	-2.244226	1.064350
0.85	-3.130826	-2.336113	1.796972
0.90	-3.233088	-2.353418	2.261226
0.95	-3.291294	-2.287005	2.502916
1.00	-3.310290	-2.239334	2.580567

K_F = 3.60 WMF = - .6308135

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	-0.000836	-0.001906	-0.003221
0.10	-0.005089	-0.012641	-0.023058
0.15	-0.017045	-0.039320	-0.068581
0.20	-0.041164	-0.081549	-0.123446
0.25	-0.079649	-0.134791	-0.169191
0.30	-0.131796	-0.198882	-0.212876
0.35	-0.196376	-0.280327	-0.266455
0.40	-0.276531	-0.382369	-0.309974
0.45	-0.384255	-0.489499	-0.285841
0.50	-0.540350	-0.576188	-0.195716
0.55	-0.767325	-0.641056	-0.066902
0.60	-1.076915	-0.706099	0.186849
0.65	-1.458313	-0.768209	0.565520
0.70	-1.874901	-0.793104	1.081713
0.75	-2.273524	-0.770399	1.864611
0.80	-2.603355	-0.708626	2.694623
0.85	-2.835284	-0.561833	3.266092
0.90	-2.970248	-0.269895	3.603158
0.95	-3.032161	0.077462	3.787573
1.00	-3.048767	0.238444	3.844571

K_F = 4.00 WMF = - 2.505328

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	-0.009396	-0.018673	-0.027809
0.10	-0.038146	-0.074150	-0.107358
0.15	-0.087113	-0.163815	-0.227995
0.20	-0.156512	-0.286461	-0.389151
0.25	-0.247466	-0.444419	-0.595173
0.30	-0.366236	-0.634515	-0.821502
0.35	-0.527305	-0.849303	-1.031964
0.40	-0.750156	-1.093699	-1.224110
0.45	-1.048367	-1.384371	-1.417228
0.50	-1.416436	-1.730265	-1.593526
0.55	-1.823693	-2.119853	-1.689324
0.60	-2.222014	-2.521983	-1.714818
0.65	-2.565038	-2.907499	-1.676538
0.70	-2.827992	-3.271854	-1.495776
0.75	-3.015718	-3.609782	-1.198487
0.80	-3.153331	-3.892365	-0.729666
0.85	-3.266142	-4.129359	-0.038477
0.90	-3.362936	-4.390590	0.577111
0.95	-3.433212	-4.664832	0.909499
1.00	-3.459320	-4.791598	1.010332

K_F = 4.20 WMF = - 3.33013

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	-0.017763	-0.035459	-0.053104
0.10	-0.065461	-0.129738	-0.193279
0.15	-0.132286	-0.258246	-0.378823
0.20	-0.215129	-0.409670	-0.583378
0.25	-0.327389	-0.600215	-0.824220
0.30	-0.495199	-0.859364	-1.126883
0.35	-0.741927	-1.203205	-1.473004
0.40	-1.070815	-1.622144	-1.821867
0.45	-1.457601	-2.091388	-2.155915
0.50	-1.858213	-2.589833	-2.475132
0.55	-2.226981	-3.101293	-2.747828
0.60	-2.533906	-3.598839	-2.912982
0.65	-2.771751	-4.053391	-2.991535
0.70	-2.950735	-4.462640	-2.979475
0.75	-3.087040	-4.844109	-2.812177
0.80	-3.193018	-5.212581	-2.533637
0.85	-3.274159	-5.597732	-2.084706
0.90	-3.331564	-6.026929	-1.471095
0.95	-3.365432	-6.421823	-1.010593
1.00	-3.376533	-6.589672	-0.868730

K_F = 4.60 WMF = - 4.390126

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	-0.012005	-0.024028	-0.036066
0.10	-0.058717	-0.116381	-0.173015
0.15	-0.164636	-0.317305	-0.459526
0.20	-0.350265	-0.650833	-0.910337
0.25	-0.615608	-1.105996	-1.490154
0.30	-0.935327	-1.640777	-2.134689
0.35	-1.268010	-2.206308	-2.800397
0.40	-1.573280	-2.770261	-3.469412
0.45	-1.826327	-3.310021	-4.106666
0.50	-2.022480	-3.799423	-4.667700
0.55	-2.171620	-4.227694	-5.142396
0.60	-2.288095	-4.615472	-5.559966
0.65	-2.383069	-4.993637	-5.916196
0.70	-2.462370	-5.392256	-6.181058
0.75	-2.528501	-5.854071	-6.391767
0.80	-2.583182	-6.396293	-6.522902
0.85	-2.627776	-6.940275	-6.541534
0.90	-2.662241	-7.346683	-6.498955
0.95	-2.684712	-7.550703	-6.331995
1.00	-2.692588	-7.603158	-6.197988

K_F = 4.40 WMF = - 3.947657

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	-0.014816	-0.029588	-0.044309
0.10	-0.059112	-0.117720	-0.175601
0.15	-0.135274	-0.266826	-0.394319
0.20	-0.253100	-0.483834	-0.695244
0.25	-0.429333	-0.778033	-1.062715
0.30	-0.678155	-1.163816	-1.501330
0.35	-0.997416	-1.648295	-2.019445
0.40	-1.360987	-2.207647	-2.573658
0.45	-1.725057	-2.792688	-3.095598
0.50	-2.046488	-3.356860	-3.557640
0.55	-2.301944	-3.873672	-3.969634
0.60	-2.495093	-4.342360	-4.304860
0.65	-2.647332	-4.772726	-4.509190
0.70	-2.779426	-5.164149	-4.618328
0.75	-2.897486	-5.540955	-4.628864
0.80	-2.992928	-5.981310	-4.493894
0.85	-3.054367	-6.510783	-4.256922
0.90	-3.080887	-7.002213	-3.852490
0.95	-3.085099	-7.302679	-3.362401
1.00	-3.083934	-7.392343	-3.141335

K_F = 4.80 WMF = - 4.679273

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	-0.030166	-0.059799	-0.088920
0.10	-0.126057	-0.244443	-0.355941
0.15	-0.296858	-0.561854	-0.798621
0.20	-0.540423	-1.006059	-1.401597
0.25	-0.832912	-1.542300	-2.121835
0.30	-1.132755	-2.107156	-2.878111
0.35	-1.397585	-2.635477	-3.588277
0.40	-1.602798	-3.093185	-4.233593
0.45	-1.749019	-3.484839	-4.837545
0.50	-1.854302	-3.838487	-5.396196
0.55	-1.938040	-4.180416	-5.895007
0.60	-2.008686	-4.522233	-6.355490
0.65	-2.063334	-4.893423	-6.820977
0.70	-2.096964	-5.362638	-7.276595
0.75	-2.111922	-5.946331	-7.704459
0.80	-2.119141	-6.521315	-8.169282
0.85	-2.130468	-6.940619	-8.652094
0.90	-2.149436	-7.199924	-9.102744
0.95	-2.168675	-7.368185	-9.513431
1.00	-2.176853	-7.435442	-9.702718

K_F = 5.00 WMF = - 4.590907

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	-0.054400	-0.108222	-0.161448
0.10	-0.204705	-0.402598	-0.592979
0.15	-0.417203	-0.813660	-1.184827
0.20	-0.649789	-1.269044	-1.841472
0.25	-0.865767	-1.715784	-2.504085
0.30	-1.042958	-2.128547	-3.149759
0.35	-1.175368	-2.497525	-3.759996
0.40	-1.268576	-2.814660	-4.307201
0.45	-1.332960	-3.089864	-4.805655
0.50	-1.378274	-3.359845	-5.312395
0.55	-1.411216	-3.658669	-5.851654
0.60	-1.435294	-4.012192	-6.406502
0.65	-1.451551	-4.457690	-6.985334
0.70	-1.459418	-4.999677	-7.648201
0.75	-1.457591	-5.550566	-8.406150
0.80	-1.445685	-5.991271	-9.236808
0.85	-1.425804	-6.284383	-10.124746
0.90	-1.403253	-6.470443	-10.973928
0.95	-1.385354	-6.584026	-11.701994
1.00	-1.378558	-6.624031	-12.032342

K_F = 5.40 WMF = - 2.482063

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	-0.006639	-0.014204	-0.022694
0.10	-0.020855	-0.054664	-0.101435
0.15	-0.028631	-0.111507	-0.247683
0.20	-0.014991	-0.167341	-0.448046
0.25	0.028866	-0.205732	-0.672335
0.30	0.102684	-0.222636	-0.906810
0.35	0.199574	-0.239879	-1.183486
0.40	0.311381	-0.296831	-1.565211
0.45	0.433069	-0.418496	-2.067909
0.50	0.563427	-0.619815	-2.658947
0.55	0.702244	-0.931552	-3.363536
0.60	0.846527	-1.353101	-4.264649
0.65	0.988689	-1.794095	-5.367995
0.70	1.118060	-2.147043	-6.556373
0.75	1.224646	-2.393231	-7.698842
0.80	1.302870	-2.570899	-8.752501
0.85	1.353164	-2.699057	-9.726147
0.90	1.380896	-2.788110	-10.519973
0.95	1.393440	-2.851637	-10.984757
1.00	1.396841	-2.877851	-11.122308

K_F = 5.20 WMF = - 3.833371

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	-0.048217	-0.096932	-0.146136
0.10	-0.173731	-0.354169	-0.540640
0.15	-0.329408	-0.686137	-1.064004
0.20	-0.464403	-1.000428	-1.584470
0.25	-0.547412	-1.247938	-2.042318
0.30	-0.575654	-1.434659	-2.458311
0.35	-0.566760	-1.596411	-2.879090
0.40	-0.541953	-1.770929	-3.323739
0.45	-0.512913	-1.977385	-3.790436
0.50	-0.479822	-2.216268	-4.301877
0.55	-0.438670	-2.509114	-4.895190
0.60	-0.389619	-2.912137	-5.586633
0.65	-0.339173	-3.428841	-6.394734
0.70	-0.295488	-3.942078	-7.350211
0.75	-0.262108	-4.324933	-8.440954
0.80	-0.236166	-4.584292	-9.532199
0.85	-0.212454	-4.794229	-10.529617
0.90	-0.189336	-4.951924	-11.452526
0.95	-0.170954	-5.019440	-12.086208
1.00	-0.163823	-5.029026	-12.275685

K_F = 5.60 WMF = - 1.050404

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	0.039518	0.078582	0.117187
0.10	0.145579	0.283004	0.412042
0.15	0.287682	0.532962	0.734260
0.20	0.433770	0.746505	0.932777
0.25	0.565842	0.888160	0.957067
0.30	0.685604	0.965009	0.835728
0.35	0.808085	0.997335	0.596389
0.40	0.949011	0.998147	0.236610
0.45	1.114723	0.941745	-0.278488
0.50	1.300347	0.767421	-0.995011
0.55	1.495312	0.472379	-1.932690
0.60	1.690595	0.162284	-3.059379
0.65	1.882072	-0.062770	-4.262691
0.70	2.068496	-0.217875	-5.390575
0.75	2.247064	-0.360064	-6.371923
0.80	2.410834	-0.480970	-7.309426
0.85	2.549837	-0.548376	-8.201646
0.90	2.654692	-0.582030	-8.822200
0.95	2.719247	-0.614159	-9.175443
1.00	2.740897	-0.631338	-9.316923

K_F = 5.80 WMF = -.1134803

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	0.055807	0.111265	0.166375
0.10	0.206114	0.407682	0.604692
0.15	0.408429	0.798448	1.168126
0.20	0.615936	1.179421	1.678227
0.25	0.797975	1.467193	1.977026
0.30	0.948554	1.630845	2.002220
0.35	1.080187	1.695270	1.802022
0.40	1.209667	1.685024	1.431701
0.45	1.346462	1.583102	0.847624
0.50	1.490383	1.391297	-0.031394
0.55	1.637440	1.191735	-1.143252
0.60	1.787148	1.073975	-2.273881
0.65	1.944548	1.037665	-3.276414
0.70	2.115745	1.031561	-4.173281
0.75	2.300840	1.032462	-5.086116
0.80	2.489927	1.032006	-5.987951
0.85	2.665181	1.017960	-6.671588
0.90	2.806600	1.005260	-7.114450
0.95	2.897918	1.015263	-7.354351
1.00	2.929290	1.026532	-7.412739

K_F = 6.20 WMF = - 8.554401E-02

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	0.008738	0.018025	0.027856
0.10	0.043584	0.092769	0.147615
0.15	0.122449	0.258290	0.409631
0.20	0.254758	0.524792	0.816888
0.25	0.427723	0.860180	1.303948
0.30	0.607434	1.165848	1.684485
0.35	0.754460	1.308236	1.696581
0.40	0.842855	1.244183	1.234631
0.45	0.869417	1.079180	0.480367
0.50	0.847797	0.947808	-0.267596
0.55	0.793395	0.890548	-0.884881
0.60	0.711068	0.886430	-1.466905
0.65	0.594526	0.929245	-2.146615
0.70	0.436437	1.022477	-2.910907
0.75	0.240539	1.155460	-3.547432
0.80	0.026202	1.314542	-3.983724
0.85	-0.177204	1.480601	-4.318916
0.90	-0.341086	1.616132	-4.541872
0.95	-0.445658	1.691805	-4.688183
1.00	-0.481253	1.713110	-4.760197

K_F = 6.00 WMF = .1246895

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	0.034714	0.069661	0.104832
0.10	0.135798	0.275005	0.417088
0.15	0.293053	0.598051	0.911455
0.20	0.487574	0.988118	1.492661
0.25	0.692894	1.362793	1.991148
0.30	0.880671	1.641715	2.246022
0.35	1.029395	1.764484	2.170417
0.40	1.131572	1.700352	1.733014
0.45	1.195076	1.499535	0.970878
0.50	1.237578	1.298878	0.018602
0.55	1.277195	1.201677	-0.948083
0.60	1.324528	1.194767	-1.813496
0.65	1.380116	1.231721	-2.576216
0.70	1.437561	1.313496	-3.367580
0.75	1.489121	1.438803	-4.234226
0.80	1.530039	1.563518	-4.953612
0.85	1.559502	1.650005	-5.420488
0.90	1.578978	1.698904	-5.734847
0.95	1.590108	1.723538	-5.915865
1.00	1.593735	1.731044	-5.968007

K_F = 6.40 WMF = - .4256871

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	0.002705	0.004816	0.006369
0.10	0.012921	0.019390	0.020610
0.15	0.036384	0.056614	0.065469
0.20	0.080355	0.142624	0.195002
0.25	0.149486	0.274774	0.399263
0.30	0.240434	0.403241	0.550873
0.35	0.337745	0.489183	0.512369
0.40	0.414179	0.546913	0.277844
0.45	0.436863	0.590898	-0.042362
0.50	0.377470	0.596389	-0.371692
0.55	0.221859	0.557902	-0.720207
0.60	-0.025364	0.521270	-1.160311
0.65	-0.343221	0.516973	-1.746047
0.70	-0.701563	0.529144	-2.304587
0.75	-1.068742	0.553628	-2.680395
0.80	-1.416140	0.618765	-2.957323
0.85	-1.718934	0.735576	-3.166900
0.90	-1.955114	0.874455	-3.304991
0.95	-2.105790	0.987472	-3.372664
1.00	-2.157481	1.031179	-3.381213

K_F = 6.60 WMF = - .7991163

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	-0.002346	-0.004895	-0.007688
0.10	-0.012759	-0.027251	-0.044923
0.15	-0.037045	-0.079327	-0.132281
0.20	-0.074872	-0.173620	-0.293763
0.25	-0.116258	-0.312608	-0.552819
0.30	-0.148697	-0.438301	-0.825992
0.35	-0.171183	-0.441873	-0.917626
0.40	-0.204024	-0.290786	-0.751327
0.45	-0.284848	-0.090583	-0.506101
0.50	-0.450718	0.032250	-0.419650
0.55	-0.716953	0.045097	-0.571763
0.60	-1.066480	-0.017823	-0.904744
0.65	-1.456687	-0.118784	-1.239314
0.70	-1.838869	-0.227579	-1.473212
0.75	-2.177275	-0.322092	-1.680525
0.80	-2.456612	-0.393217	-1.834347
0.85	-2.676024	-0.435453	-1.916955
0.90	-2.837500	-0.445572	-1.981728
0.95	-2.938417	-0.435507	-2.005380
1.00	-2.972967	-0.428280	-2.001611

K_F = 7.00 WMF = - 1.29312

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	-0.023759	-0.048818	-0.075114
0.10	-0.097671	-0.212184	-0.341308
0.15	-0.229534	-0.512784	-0.842953
0.20	-0.430487	-0.918888	-1.486123
0.25	-0.708973	-1.336398	-2.033516
0.30	-1.060991	-1.689741	-2.294412
0.35	-1.461873	-1.966747	-2.253047
0.40	-1.866749	-2.153216	-1.963573
0.45	-2.222984	-2.200170	-1.458333
0.50	-2.489857	-2.101989	-0.885357
0.55	-2.654780	-1.937823	-0.412524
0.60	-2.736096	-1.803074	-0.050160
0.65	-2.770478	-1.751929	0.200043
0.70	-2.792846	-1.806363	0.408819
0.75	-2.821119	-1.964204	0.637979
0.80	-2.854160	-2.196515	0.806817
0.85	-2.881600	-2.463925	0.919712
0.90	-2.896370	-2.725129	1.008012
0.95	-2.900380	-2.924421	1.058588
1.00	-2.900510	-3.000018	1.076150

K_F = 6.8 WMF = - 1.137133

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	-0.014710	-0.028703	-0.041971
0.10	-0.058490	-0.111906	-0.159550
0.15	-0.131255	-0.267329	-0.401358
0.20	-0.234985	-0.528398	-0.860055
0.25	-0.374125	-0.860120	-1.457046
0.30	-0.553281	-1.139019	-1.897545
0.35	-0.773270	-1.263197	-1.925609
0.40	-1.028248	-1.233799	-1.552470
0.45	-1.306220	-1.112452	-1.021951
0.50	-1.592671	-0.967414	-0.609340
0.55	-1.874873	-0.874621	-0.489035
0.60	-2.143839	-0.892879	-0.569456
0.65	-2.392933	-1.008269	-0.617803
0.70	-2.615173	-1.153799	-0.618190
0.75	-2.802047	-1.296448	-0.611484
0.80	-2.945857	-1.461277	-0.592396
0.85	-3.043854	-1.666756	-0.580160
0.90	-3.100886	-1.878456	-0.565587
0.95	-3.127669	-2.034990	-0.580249
1.00	-3.135074	-2.091712	-0.604055

K_F = 7.20 WMF = - 1.127951

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	-0.047684	-0.096426	-0.146316
0.10	-0.191743	-0.389011	-0.596069
0.15	-0.431932	-0.833059	-1.236429
0.20	-0.759293	-1.310769	-1.775217
0.25	-1.149981	-1.735837	-2.033253
0.30	-1.565246	-2.108452	-2.080774
0.35	-1.958655	-2.431207	-2.025914
0.40	-2.287399	-2.657920	-1.851566
0.45	-2.522428	-2.746637	-1.520674
0.50	-2.653503	-2.689861	-0.997693
0.55	-2.688385	-2.499443	-0.237062
0.60	-2.648150	-2.232386	0.589348
0.65	-2.561020	-2.014184	1.268469
0.70	-2.456639	-1.963535	1.774755
0.75	-2.360717	-2.089043	2.143915
0.80	-2.290474	-2.296050	2.444152
0.85	-2.251579	-2.487179	2.676674
0.90	-2.238488	-2.625658	2.829130
0.95	-2.238798	-2.711568	2.949207
1.00	-2.240527	-2.741773	3.004895

K_F = 7.40 WMF = -. 3353624

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	-0.076468	-0.148596	-0.216459
0.10	-0.289428	-0.519308	-0.693562
0.15	-0.594647	-0.955833	-1.112627
0.20	-0.933659	-1.346901	-1.316996
0.25	-1.250952	-1.665848	-1.344228
0.30	-1.508471	-1.910396	-1.276915
0.35	-1.691869	-2.068945	-1.143427
0.40	-1.806526	-2.149885	-0.979569
0.45	-1.866233	-2.173331	-0.778179
0.50	-1.881248	-2.125082	-0.324191
0.55	-1.852535	-1.981727	0.508101
0.60	-1.775268	-1.777383	1.577479
0.65	-1.648383	-1.588120	2.651614
0.70	-1.483194	-1.463047	3.497324
0.75	-1.304292	-1.409476	4.095523
0.80	-1.141483	-1.412579	4.561003
0.85	-1.017553	-1.434554	4.919206
0.90	-0.939873	-1.430508	5.163207
0.95	-0.901496	-1.396659	5.293149
1.00	-0.890588	-1.376074	5.329653

K_F = 7.80 WMF = 3.554914

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	0.057217	0.110578	0.160239
0.10	0.212479	0.375995	0.498179
0.15	0.424678	0.678014	0.814918
0.20	0.647430	0.957065	1.098769
0.25	0.848785	1.202245	1.409173
0.30	1.020696	1.401518	1.718234
0.35	1.174630	1.556105	1.984780
0.40	1.328314	1.686633	2.349366
0.45	1.492935	1.782351	2.936484
0.50	1.668484	1.802299	3.669081
0.55	1.848360	1.762881	4.513921
0.60	2.028135	1.769477	5.507808
0.65	2.211324	1.927564	6.704845
0.70	2.407818	2.258581	8.052222
0.75	2.625945	2.708134	9.300008
0.80	2.863155	3.185765	10.264205
0.85	3.101369	3.588940	10.934847
0.90	3.309510	3.843983	11.390969
0.95	3.452673	3.953338	11.688297
1.00	3.503618	3.977628	11.796827

K_F = 7.60 WMF = 1.387561

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	-0.038618	-0.072812	-0.102531
0.10	-0.140446	-0.227805	-0.258760
0.15	-0.269761	-0.370917	-0.272123
0.20	-0.384807	-0.480165	-0.166724
0.25	-0.454704	-0.551951	-0.026060
0.30	-0.469265	-0.559313	0.176745
0.35	-0.437780	-0.508831	0.427049
0.40	-0.378883	-0.444083	0.651173
0.45	-0.307977	-0.386069	0.968810
0.50	-0.229060	-0.339198	1.516286
0.55	-0.134509	-0.315272	2.303460
0.60	-0.011633	-0.287597	3.355460
0.65	0.148424	-0.177259	4.561446
0.70	0.344251	0.058153	5.723145
0.75	0.562895	0.362393	6.682086
0.80	0.783321	0.637244	7.366189
0.85	0.982142	0.828968	7.861589
0.90	1.138782	0.943570	8.213360
0.95	1.238375	1.005426	8.389339
1.00	1.272364	1.025695	8.432285

K_F = 8.00 WMF = 5.041087

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	0.093155	0.180935	0.263306
0.10	0.352951	0.637020	0.850025
0.15	0.727145	1.206274	1.422778
0.20	1.148509	1.777909	1.872470
0.25	1.556196	2.284881	2.238051
0.30	1.912399	2.676677	2.499689
0.35	2.207991	2.940772	2.770969
0.40	2.455983	3.090678	3.255341
0.45	2.677384	3.147111	3.940181
0.50	2.887551	3.168562	4.770063
0.55	3.089943	3.241311	5.719232
0.60	3.279557	3.406434	6.771332
0.65	3.451996	3.655695	7.974158
0.70	3.610728	3.997226	9.317143
0.75	3.766613	4.454053	10.711776
0.80	3.929551	4.997507	11.974212
0.85	4.097655	5.534184	12.909842
0.90	4.252398	5.962852	13.513855
0.95	4.363932	6.226059	13.885230
1.00	4.404637	6.312518	14.022594

K_F = 8.20 WMF = 5.399791

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	0.050531	0.102404	0.155430
0.10	0.208074	0.425186	0.644042
0.15	0.482434	0.947589	1.355711
0.20	0.869541	1.566572	1.982724
0.25	1.338399	2.181185	2.326827
0.30	1.834069	2.729294	2.552018
0.35	2.296368	3.137625	2.901309
0.40	2.682826	3.363178	3.363296
0.45	2.981269	3.482141	3.934950
0.50	3.205390	3.629167	4.676064
0.55	3.378063	3.860838	5.581397
0.60	3.515053	4.146084	6.636246
0.65	3.619040	4.452483	7.780097
0.70	3.685516	4.787411	9.031921
0.75	3.713054	5.179133	10.446432
0.80	3.709346	5.647834	11.898828
0.85	3.688984	6.177517	13.149649
0.90	3.666501	6.697004	14.002572
0.95	3.650944	7.088691	14.426159
1.00	3.645608	7.235366	14.540164

K_F = 8.60 WMF = 4.456084

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	0.021636	0.042045	0.061108
0.10	0.080671	0.149669	0.201925
0.15	0.165936	0.309251	0.412709
0.20	0.274451	0.531496	0.831764
0.25	0.419272	0.805766	1.515135
0.30	0.622865	1.130095	2.198783
0.35	0.898860	1.568671	2.709889
0.40	1.234978	2.167387	3.160852
0.45	1.590326	2.848027	3.591261
0.50	1.910176	3.478096	3.997051
0.55	2.149100	3.997106	4.410382
0.60	2.287519	4.420278	4.892630
0.65	2.332628	4.778314	5.523401
0.70	2.306210	5.088857	6.294514
0.75	2.230443	5.349481	7.185610
0.80	2.122118	5.548818	8.242618
0.85	1.996867	5.691908	9.470387
0.90	1.875995	5.796825	10.718113
0.95	1.786844	5.867974	11.693639
1.00	1.753929	5.894017	12.069340

K_F = 8.40 WMF = 5.090093

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	0.023569	0.048903	0.076197
0.10	0.100600	0.221931	0.370241
0.15	0.247643	0.552887	0.929672
0.20	0.484042	1.015834	1.556627
0.25	0.820292	1.529973	2.041306
0.30	1.245956	2.023207	2.450397
0.35	1.723796	2.477229	2.861402
0.40	2.195851	2.911373	3.283469
0.45	2.601254	3.331663	3.754502
0.50	2.897765	3.714997	4.306958
0.55	3.075143	4.052033	4.989988
0.60	3.152107	4.374380	5.799700
0.65	3.159482	4.712171	6.737071
0.70	3.120566	5.053640	7.831052
0.75	3.042580	5.378454	9.079697
0.80	2.924139	5.707749	10.474242
0.85	2.771948	6.081501	11.887043
0.90	2.612806	6.484918	13.034835
0.95	2.489751	6.816824	13.698166
1.00	2.443366	6.946967	13.894601

K_F = 8.80 WMF = 3.565308

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	0.001807	0.002723	0.002666
0.10	0.007674	0.002658	-0.013089
0.15	0.017085	-0.011299	-0.021285
0.20	0.026004	-0.007236	0.197574
0.25	0.029240	0.106448	0.774025
0.30	0.029068	0.398884	1.533919
0.35	0.043843	0.848281	2.227031
0.40	0.106742	1.405527	2.726690
0.45	0.250313	2.063165	3.105259
0.50	0.483840	2.801980	3.424317
0.55	0.778925	3.532386	3.692670
0.60	1.075886	4.144156	3.976535
0.65	1.310348	4.583473	4.288848
0.70	1.444633	4.865625	4.637130
0.75	1.484063	5.032622	5.071411
0.80	1.467804	5.096637	5.616638
0.85	1.441504	5.031569	6.316761
0.90	1.431176	4.843688	7.191604
0.95	1.435643	4.632344	8.024407
1.00	1.439850	4.539832	8.379763

K_F = 9.00 WMF = 2.66247

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	-0.024581	-0.048483	-0.071013
0.10	-0.092074	-0.172728	-0.215804
0.15	-0.187854	-0.312106	-0.261785
0.20	-0.297457	-0.373890	-0.154424
0.25	-0.411500	-0.266018	0.125321
0.30	-0.522100	0.035575	0.704586
0.35	-0.613982	0.464169	1.452365
0.40	-0.659359	0.944007	2.068488
0.45	-0.624060	1.475330	2.468077
0.50	-0.483812	2.099497	2.745159
0.55	-0.240624	2.800414	2.969761
0.60	0.072446	3.479728	3.101944
0.65	0.402885	4.021588	3.130247
0.70	0.700284	4.359881	3.117521
0.75	0.934825	4.489431	3.104153
0.80	1.102422	4.435299	3.090625
0.85	1.215845	4.231902	3.085901
0.90	1.290362	3.942209	3.114704
0.95	1.334336	3.680218	3.156416
1.00	1.349124	3.574040	3.173246

K_F = 9.40 WMF = 1.823654

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	0.002545	0.006671	0.011596
0.10	0.007916	0.037017	0.056418
0.15	0.012181	0.106052	0.119442
0.20	0.015353	0.214878	0.246925
0.25	0.023601	0.358679	0.458921
0.30	0.044706	0.545917	0.705495
0.35	0.079934	0.804545	1.071837
0.40	0.119970	1.151653	1.636014
0.45	0.150561	1.540913	2.244158
0.50	0.165956	1.879132	2.582352
0.55	0.180919	2.132483	2.546096
0.60	0.231237	2.369853	2.287274
0.65	0.359579	2.658731	1.869304
0.70	0.593591	2.968947	1.235233
0.75	0.928800	3.217396	0.365848
0.80	1.326081	3.364093	-0.728262
0.85	1.724194	3.436290	-2.030439
0.90	2.059167	3.484557	-3.402612
0.95	2.280260	3.529364	-4.502259
1.00	2.356968	3.550096	-4.927513

K_F = 9.20 WMF = 2.065495

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	-0.030476	-0.056791	-0.079594
0.10	-0.118148	-0.177266	-0.209292
0.15	-0.249691	-0.257438	-0.254790
0.20	-0.399593	-0.232952	-0.199705
0.25	-0.533739	-0.107230	-0.021922
0.30	-0.621462	0.119130	0.330962
0.35	-0.649553	0.474014	0.919290
0.40	-0.627109	0.934878	1.634245
0.45	-0.575038	1.412135	2.187042
0.50	-0.505876	1.854424	2.483094
0.55	-0.408836	2.296334	2.582930
0.60	-0.253176	2.777887	2.508920
0.65	-0.010049	3.269241	2.301475
0.70	0.321572	3.672522	1.991541
0.75	0.704026	3.874907	1.558252
0.80	1.074446	3.838704	0.989551
0.85	1.374282	3.655746	0.266214
0.90	1.574720	3.475021	-0.619079
0.95	1.680659	3.377177	-1.445387
1.00	1.712357	3.351542	-1.792436

K_F = 9.60 WMF = 1.540099

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	0.040788	0.076661	0.108908
0.10	0.157738	0.251026	0.333396
0.15	0.333155	0.430496	0.596087
0.20	0.535805	0.589895	0.856466
0.25	0.725878	0.753235	1.074320
0.30	0.868017	0.915666	1.289871
0.35	0.946395	1.051002	1.481151
0.40	0.971555	1.175586	1.698695
0.45	0.972857	1.339244	2.024373
0.50	0.980939	1.551699	2.309608
0.55	1.012550	1.761030	2.320474
0.60	1.068878	1.910189	1.982542
0.65	1.147619	1.997424	1.321746
0.70	1.257139	2.089751	0.349803
0.75	1.418103	2.281007	-0.902619
0.80	1.647453	2.607506	-2.377680
0.85	1.934764	2.993435	-3.921285
0.90	2.229821	3.306662	-5.223096
0.95	2.455052	3.476179	-6.028257
1.00	2.539392	3.523317	-6.288757

$K_F = 9.80$ WMF = .7788516

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	0.035280	0.069566	0.102855
0.10	0.141336	0.263387	0.369453
0.15	0.314560	0.519211	0.676516
0.20	0.539076	0.738633	0.936478
0.25	0.783348	0.864432	1.149369
0.30	1.007912	0.911352	1.300684
0.35	1.181296	0.900856	1.359776
0.40	1.293934	0.835899	1.304881
0.45	1.360247	0.764516	1.226561
0.50	1.407189	0.769442	1.280649
0.55	1.457251	0.846507	1.316208
0.60	1.517444	0.887642	0.956581
0.65	1.580809	0.838078	0.094990
0.70	1.637041	0.793610	-1.111252
0.75	1.682808	0.900787	-2.550355
0.80	1.723426	1.216204	-4.093880
0.85	1.765700	1.676527	-5.464684
0.90	1.809157	2.149558	-6.408577
0.95	1.843948	2.497108	-6.875440
1.00	1.857410	2.623379	-6.998288

$K_F = 10.20$ WMF = - 1.894236

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	0.003059	0.004669	0.005573
0.10	0.006657	0.000223	0.005718
0.15	0.000086	-0.015856	0.030136
0.20	-0.019301	-0.004030	0.002728
0.25	-0.036659	0.026406	-0.176916
0.30	-0.022529	-0.006425	-0.431650
0.35	0.052408	-0.141680	-0.700950
0.40	0.199731	-0.340870	-0.945915
0.45	0.403895	-0.596988	-1.236881
0.50	0.626303	-0.953177	-1.761698
0.55	0.819204	-1.377039	-2.485706
0.60	0.940674	-1.738549	-3.192290
0.65	0.963589	-1.958568	-3.918855
0.70	0.877747	-2.088861	-4.849824
0.75	0.689306	-2.217064	-5.861380
0.80	0.421537	-2.368520	-6.677756
0.85	0.116144	-2.521401	-7.235266
0.90	-0.169545	-2.653720	-7.620759
0.95	-0.373657	-2.747608	-7.884729
1.00	-0.447591	-2.782315	-7.986681

$K_F = 10.00$ WMF = - .4303409

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	0.018963	0.039627	0.061071
0.10	0.071609	0.163289	0.238317
0.15	0.149640	0.354947	0.428583
0.20	0.249444	0.542213	0.558609
0.25	0.375897	0.632240	0.629567
0.30	0.536063	0.589584	0.609688
0.35	0.727349	0.456808	0.517218
0.40	0.930848	0.293282	0.360870
0.45	1.117505	0.117140	0.133321
0.50	1.263780	-0.080623	-0.121576
0.55	1.364358	-0.290445	-0.405835
0.60	1.430621	-0.478327	-0.887359
0.65	1.474622	-0.613257	-1.746605
0.70	1.491718	-0.679229	-2.954950
0.75	1.457813	-0.664871	-4.319095
0.80	1.347381	-0.552188	-5.587017
0.85	1.160937	-0.322447	-6.546767
0.90	0.941053	0.002437	-7.155891
0.95	0.761484	0.311267	-7.497786
1.00	0.692311	0.440766	-7.613628

$K_F = 10.40$ WMF = - 3.379899

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	-0.028888	-0.056205	-0.082081
0.10	-0.104130	-0.191558	-0.265390
0.15	-0.198998	-0.355529	-0.469471
0.20	-0.287680	-0.519427	-0.679719
0.25	-0.356634	-0.641892	-0.954850
0.30	-0.402600	-0.698271	-1.326539
0.35	-0.421450	-0.766065	-1.750582
0.40	-0.401268	-0.974580	-2.257887
0.45	-0.329665	-1.356543	-2.914761
0.50	-0.211988	-1.831150	-3.718783
0.55	-0.084724	-2.311376	-4.592712
0.60	-0.008770	-2.750452	-5.397952
0.65	-0.041402	-3.122248	-6.036777
0.70	-0.203326	-3.436657	-6.546522
0.75	-0.463552	-3.758013	-6.993177
0.80	-0.753960	-4.162571	-7.354448
0.85	-1.004548	-4.677154	-7.617687
0.90	-1.175532	-5.242999	-7.812249
0.95	-1.265266	-5.709014	-7.923080
1.00	-1.291700	-5.892147	-7.951322

K_F = 10.60 WMF = - 4.522391

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	-0.028993	-0.057471	-0.085893
0.10	-0.108241	-0.211119	-0.325296
0.15	-0.217779	-0.423960	-0.685728
0.20	-0.333573	-0.662038	-1.045537
0.25	-0.436944	-0.884947	-1.335584
0.30	-0.521132	-1.059226	-1.711439
0.35	-0.592385	-1.222156	-2.321390
0.40	-0.665617	-1.483322	-3.220743
0.45	-0.756920	-1.903268	-4.328937
0.50	-0.876287	-2.420327	-5.380126
0.55	-1.023385	-2.949383	-6.236302
0.60	-1.187601	-3.480451	-6.973316
0.65	-1.351756	-4.028713	-7.513249
0.70	-1.497818	-4.579501	-7.671598
0.75	-1.612286	-5.141199	-7.570567
0.80	-1.689592	-5.765915	-7.493309
0.85	-1.732692	-6.456393	-7.496175
0.90	-1.750825	-7.106233	-7.491129
0.95	-1.755483	-7.565133	-7.464020
1.00	-1.755877	-7.728561	-7.450642

K_F = 11.00 WMF = -5.915134

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	-0.017625	-0.033281	-0.047317
0.10	-0.066714	-0.112812	-0.150454
0.15	-0.140876	-0.235445	-0.330855
0.20	-0.241645	-0.460861	-0.705643
0.25	-0.384998	-0.844573	-1.375361
0.30	-0.596748	-1.381502	-2.312784
0.35	-0.898139	-2.015576	-3.393575
0.40	-1.290578	-2.650915	-4.501956
0.45	-1.749338	-3.201902	-5.542180
0.50	-2.230135	-3.686831	-6.556281
0.55	-2.683794	-4.213963	-7.534233
0.60	-3.069564	-4.856273	-8.229761
0.65	-3.361507	-5.605672	-8.478233
0.70	-3.547378	-6.418177	-8.341702
0.75	-3.626273	-7.208223	-7.881588
0.80	-3.609338	-7.839517	-7.170258
0.85	-3.522767	-8.222727	-6.478400
0.90	-3.407712	-8.398907	-6.050270
0.95	-3.312151	-8.469822	-5.852141
1.00	-3.275357	-8.490671	-5.789758

K_F = 10.80 WMF = - 5.306024

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	-0.011346	-0.025601	-0.042102
0.10	-0.049657	-0.131285	-0.221386
0.15	-0.122645	-0.329573	-0.528114
0.20	-0.231499	-0.567303	-0.911073
0.25	-0.367107	-0.828146	-1.346699
0.30	-0.518260	-1.167150	-1.898505
0.35	-0.685829	-1.587695	-2.770244
0.40	-0.889115	-2.016313	-3.934234
0.45	-1.154821	-2.437686	-5.140296
0.50	-1.492912	-2.920635	-6.241136
0.55	-1.876376	-3.493272	-7.183567
0.60	-2.242239	-4.118659	-7.890321
0.65	-2.517078	-4.789161	-8.257506
0.70	-2.652828	-5.526721	-8.203689
0.75	-2.649950	-6.300622	-7.791861
0.80	-2.553457	-7.027288	-7.303879
0.85	-2.426137	-7.628613	-6.967206
0.90	-2.318066	-8.053224	-6.774024
0.95	-2.252174	-8.286727	-6.672932
1.00	-2.230915	-8.356810	-6.644639

K_F = 11.20 WMF = - 6.321884

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	-0.006409	-0.011852	-0.016557
0.10	-0.031440	-0.053574	-0.074993
0.15	-0.092823	-0.172598	-0.276051
0.20	-0.218852	-0.466739	-0.779818
0.25	-0.441140	-0.993556	-1.660115
0.30	-0.780818	-1.691622	-2.792676
0.35	-1.234043	-2.448258	-3.851662
0.40	-1.766352	-3.197132	-4.730871
0.45	-2.321693	-3.893530	-5.634347
0.50	-2.843019	-4.493706	-6.579519
0.55	-3.293226	-5.042564	-7.381807
0.60	-3.664042	-5.668329	-7.917075
0.65	-3.968854	-6.411008	-8.137155
0.70	-4.225870	-7.155354	-8.058297
0.75	-4.443760	-7.765545	-7.713004
0.80	-4.619157	-8.185744	-7.079902
0.85	-4.745027	-8.419948	-6.253054
0.90	-4.821273	-8.511375	-5.530209
0.95	-4.857838	-8.530726	-5.123841
1.00	-4.867989	-8.531783	-5.008560

KF = 11.40 WMF = -6.650689

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	-0.003254	-0.010020	-0.019711
0.10	-0.033031	-0.106678	-0.199136
0.15	-0.137121	-0.390089	-0.664596
0.20	-0.362141	-0.869209	-1.415527
0.25	-0.725919	-1.494761	-2.339058
0.30	-1.207185	-2.223473	-3.247640
0.35	-1.756453	-2.998616	-4.073881
0.40	-2.318607	-3.760391	-4.864287
0.45	-2.852614	-4.506895	-5.693067
0.50	-3.338983	-5.264066	-6.487458
0.55	-3.775799	-6.005214	-7.052574
0.60	-4.170644	-6.681894	-7.379014
0.65	-4.535501	-7.286256	-7.564275
0.70	-4.884898	-7.809189	-7.587748
0.75	-5.232661	-8.211351	-7.399966
0.80	-5.584061	-8.490774	-7.001408
0.85	-5.926404	-8.687320	-6.348071
0.90	-6.225163	-8.805366	-5.523920
0.95	-6.432722	-8.837296	-4.874873
1.00	-6.507204	-8.833730	-4.648170

KF = 11.60 WMF = - 6.884319

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	-0.061450	-0.122026	-0.182122
0.10	-0.243403	-0.474926	-0.709271
0.15	-0.537237	-1.022152	-1.523961
0.20	-0.925371	-1.693450	-2.429943
0.25	-1.380579	-2.390659	-3.189779
0.30	-1.869782	-3.056920	-3.782965
0.35	-2.361774	-3.718105	-4.428459
0.40	-2.835198	-4.425950	-5.226603
0.45	-3.282985	-5.208455	-5.932257
0.50	-3.711051	-6.066063	-6.409276
0.55	-4.132707	-6.926825	-6.746170
0.60	-4.561728	-7.635801	-6.976705
0.65	-5.007016	-8.092991	-7.117140
0.70	-5.469432	-8.366501	-7.177006
0.75	-5.939968	-8.590846	-7.126805
0.80	-6.399000	-8.814177	-6.948174
0.85	-6.816374	-9.007979	-6.618436
0.90	-7.154716	-9.152307	-6.084792
0.95	-7.376565	-9.246248	-5.464468
1.00	-7.453732	-9.280427	-5.170566

KF = 11.80 WMF = - 6.335504

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	-0.108833	-0.214207	-0.316315
0.10	-0.408697	-0.770754	-1.094850
0.15	-0.831343	-1.484204	-2.008553
0.20	-1.295401	-2.201135	-2.808422
0.25	-1.736519	-2.850058	-3.417628
0.30	-2.124862	-3.420614	-3.980532
0.35	-2.464633	-3.970614	-4.611397
0.40	-2.780842	-4.607839	-5.216271
0.45	-3.103606	-5.372191	-5.633773
0.50	-3.457464	-6.172945	-5.808464
0.55	-3.857038	-6.888789	-5.911012
0.60	-4.305377	-7.449850	-6.063863
0.65	-4.791933	-7.814922	-6.197123
0.70	-5.291529	-7.993175	-6.299751
0.75	-5.767337	-8.082069	-6.397864
0.80	-6.180431	-8.182759	-6.450206
0.85	-6.501984	-8.318042	-6.453164
0.90	-6.721253	-8.475228	-6.403813
0.95	-6.844297	-8.624790	-6.271116
1.00	-6.883213	-8.691062	-6.183932

KF = 12.00 WMF = - 4.445015

x	E		
	100	110	111
0.00	0.000000	0.000000	0.000000
0.05	-0.076281	-0.151464	-0.225083
0.10	-0.285552	-0.553708	-0.785659
0.15	-0.577215	-1.074508	-1.395210
0.20	-0.890143	-1.582338	-1.914067
0.25	-1.175982	-2.040424	-2.477510
0.30	-1.414950	-2.506821	-3.133748
0.35	-1.618311	-3.037021	-3.679569
0.40	-1.818016	-3.621465	-3.925162
0.45	-2.049865	-4.208650	-3.968394
0.50	-2.337747	-4.734746	-3.969002
0.55	-2.684772	-5.148271	-3.942106
0.60	-3.073139	-5.455357	-3.960453
0.65	-3.470927	-5.699067	-4.088958
0.70	-3.842259	-5.865184	-4.285654
0.75	-4.157126	-5.903752	-4.526489
0.80	-4.398326	-5.863924	-4.815485
0.85	-4.563630	-5.874454	-5.134390
0.90	-4.663256	-5.971286	-5.527701
0.95	-4.713428	-6.072743	-5.999310
1.00	-4.728248	-6.110964	-6.239461

APPENDIX III

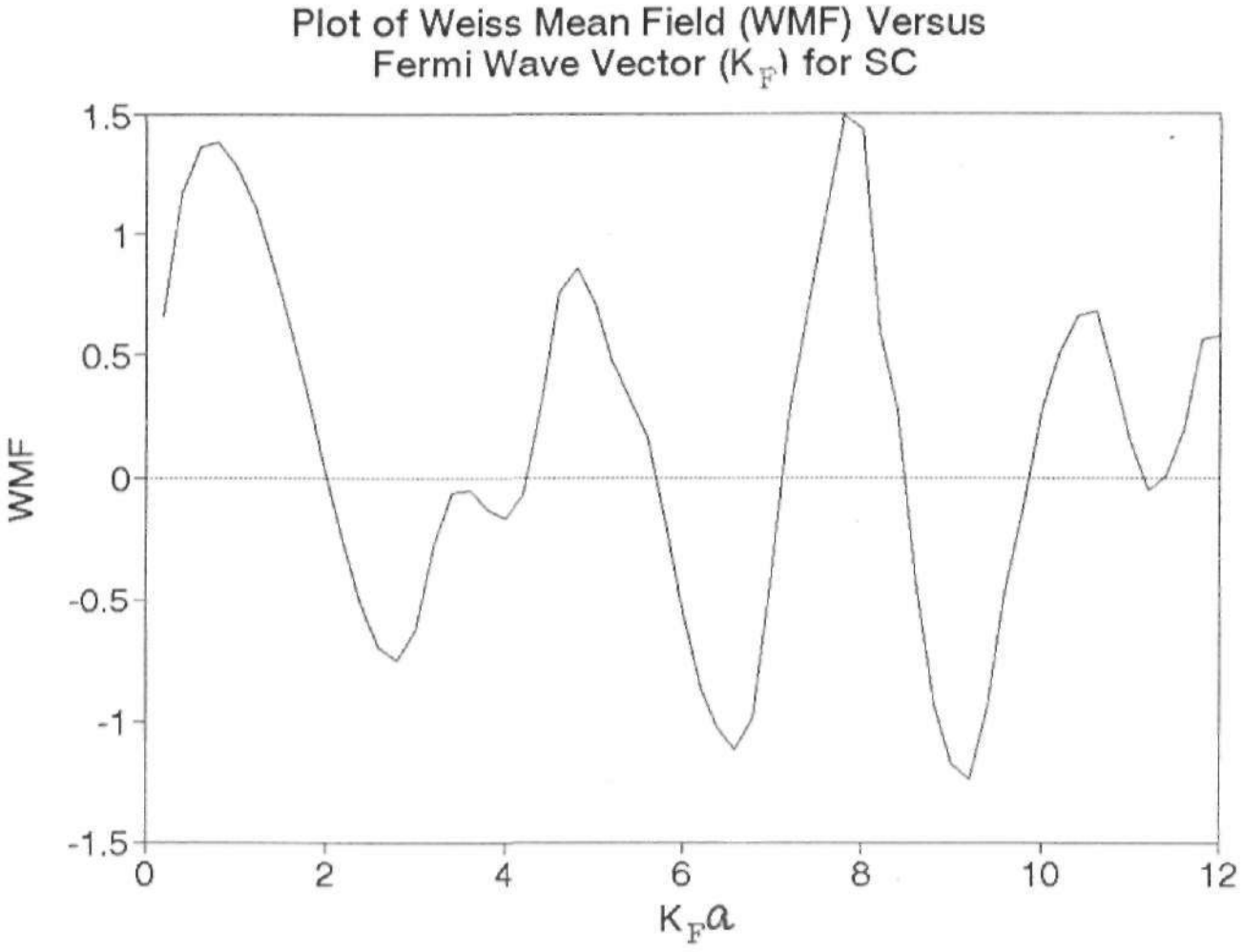


Fig A3.1

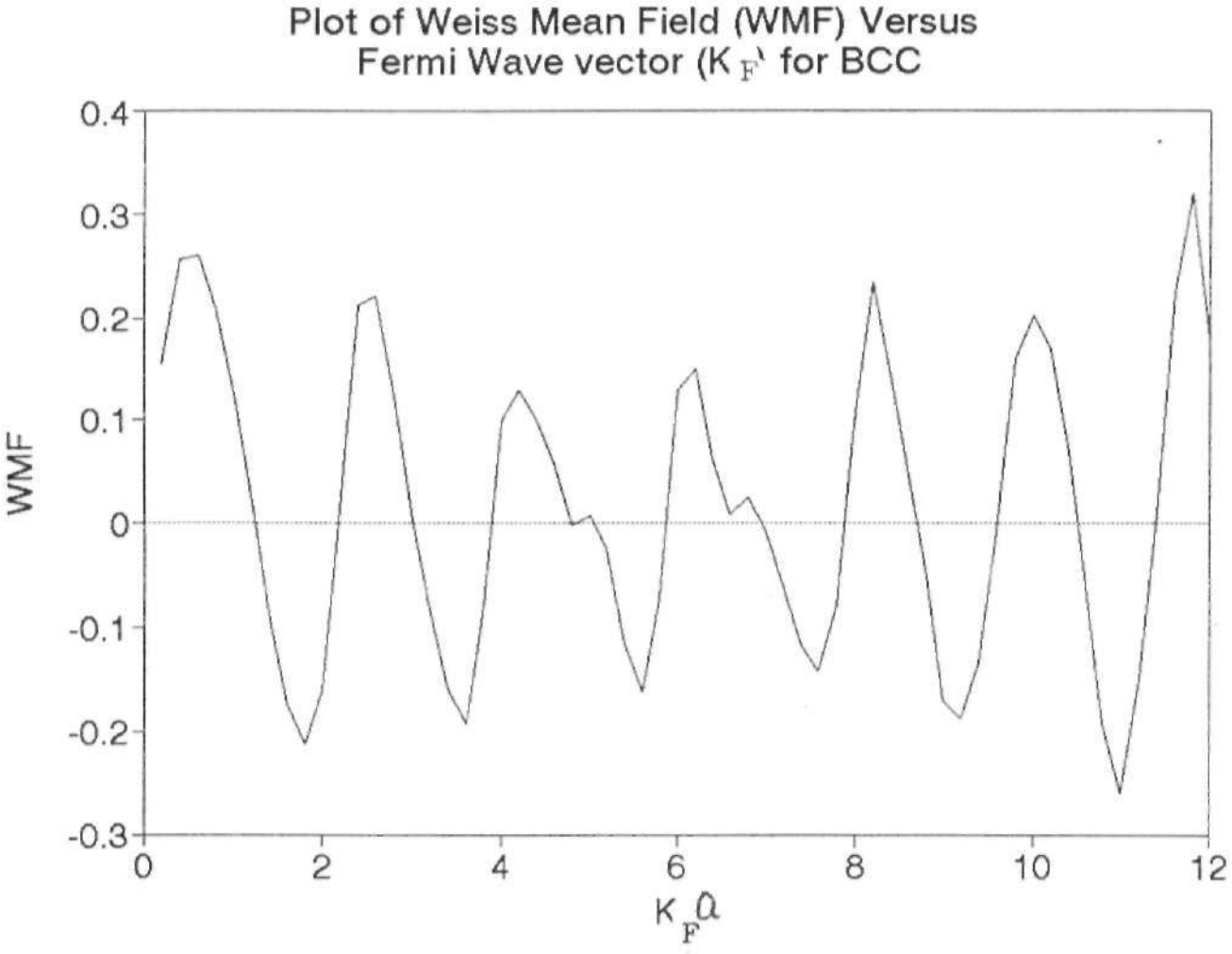

Plot of Weiss Mean Field (WMF) Versus
Fermi Wave vector (K_F) for BCC
WMF
0.4
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
0
2
4
6
8
10
12
$K_F a$

Fig A3.2

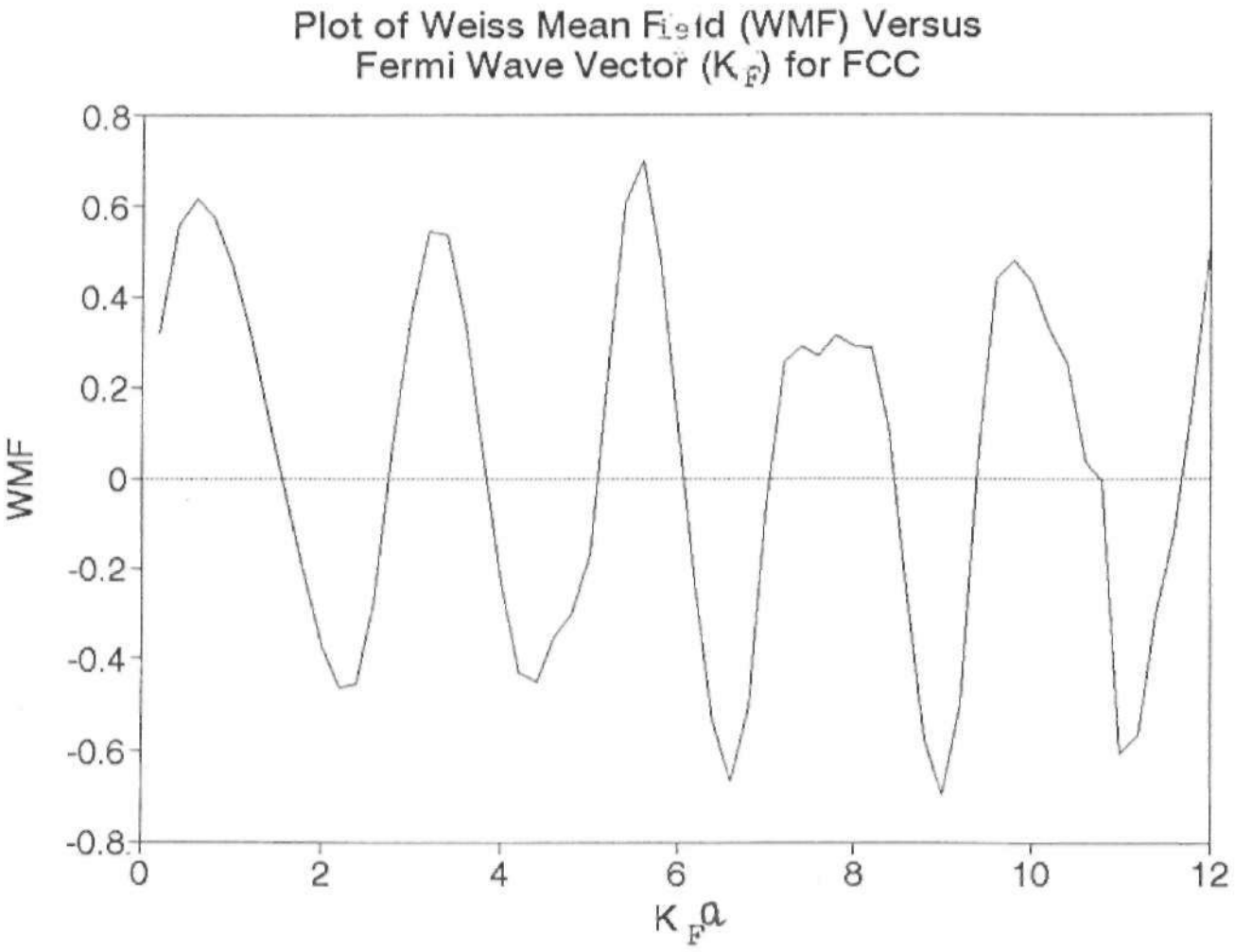

Plot of Weiss Mean Field (WMF) Versus
Fermi Wave Vector (K_F) for FCC
WMF
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
0
2
4
6
8
10
12
$K_F a$

Fig A3.3

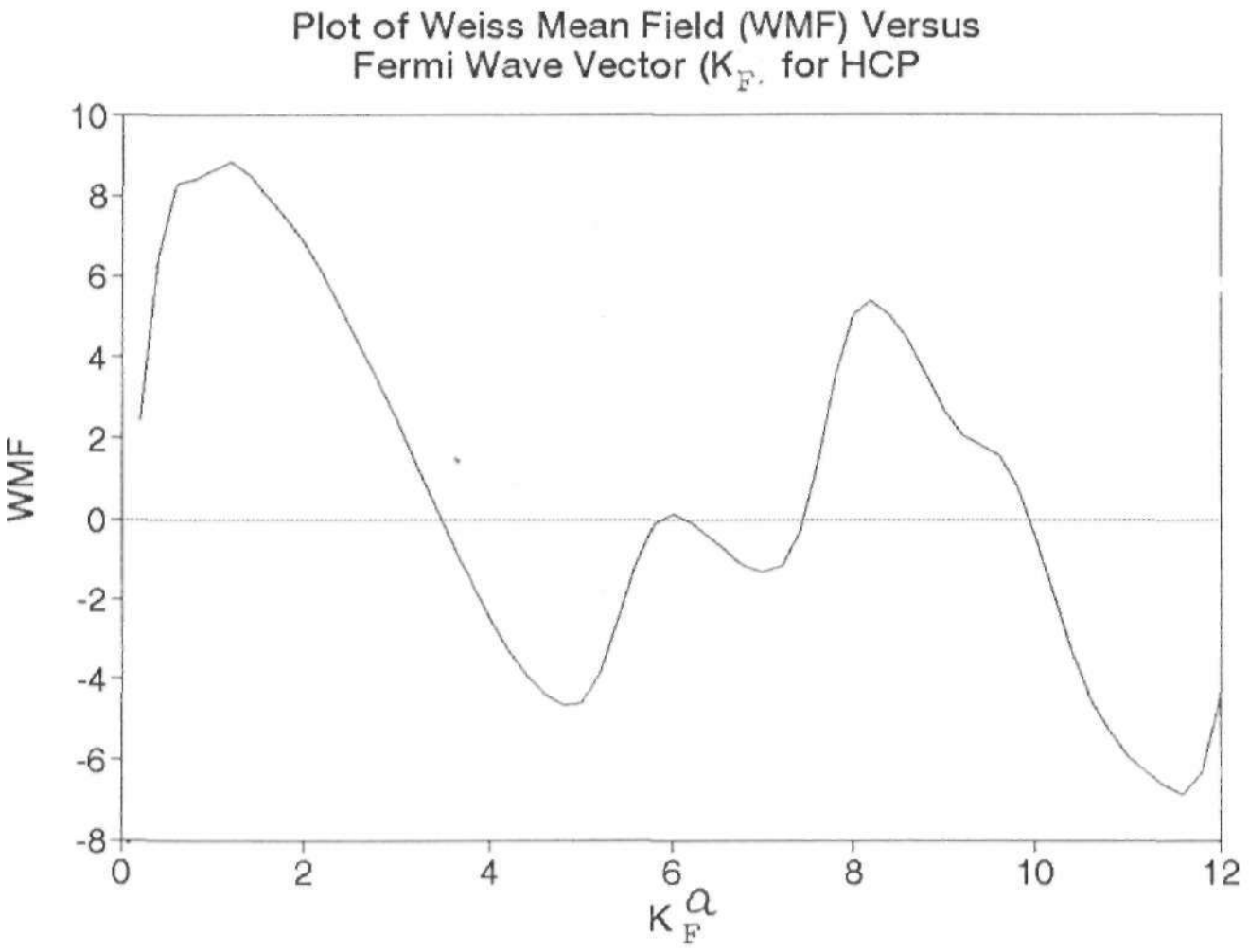

Plot of Weiss Mean Field (WMF) Versus
Fermi Wave Vector (K_F. for HCP
WMF
10
8
6
4
2
0
-2
-4
-6
-8
0
2
4
6
8
10
12
$K_F a$

Fig A3.4

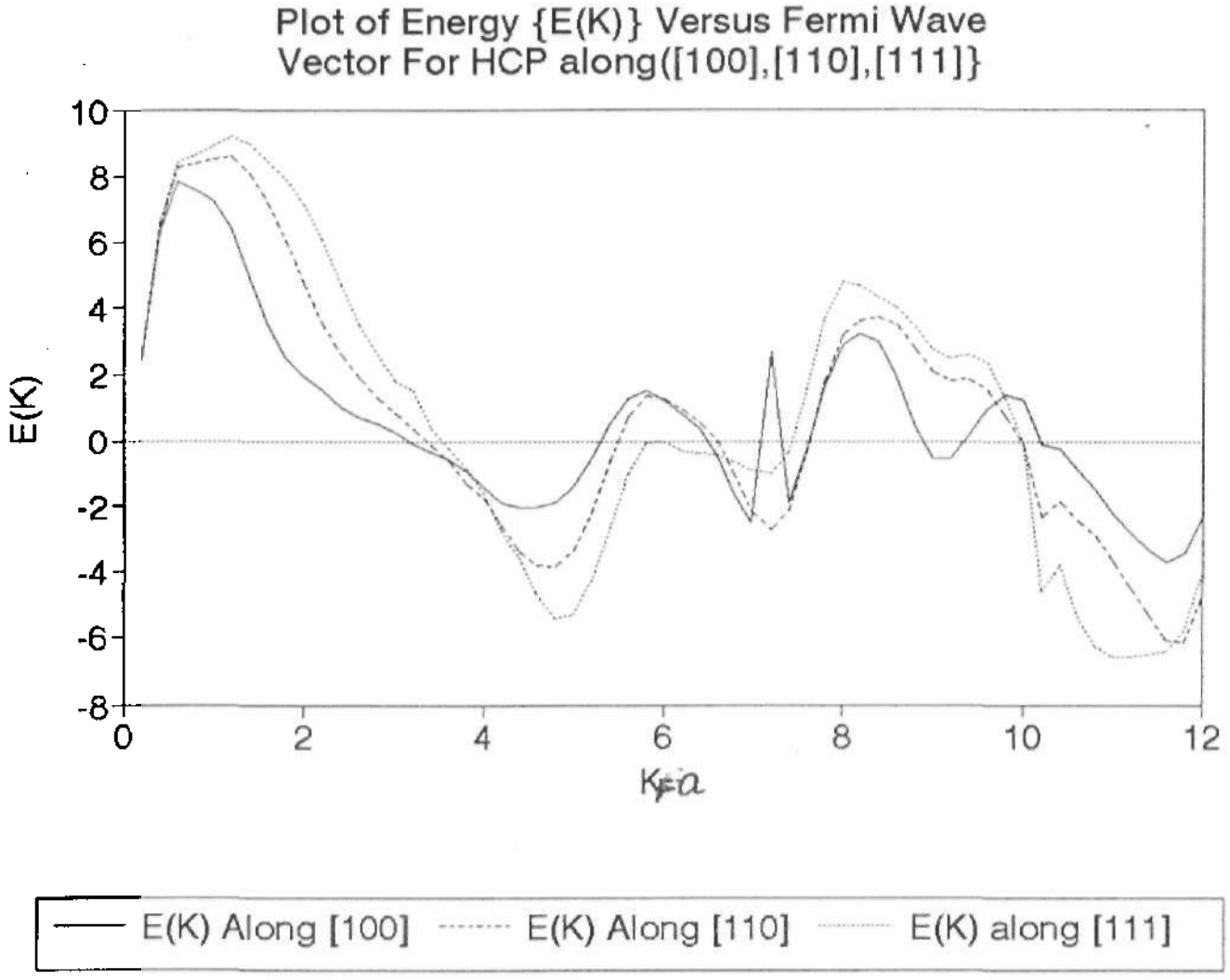

Plot of Energy {E(K)} Versus Fermi Wave Vector For HCP along([100],[110],[111]}
E(K)
10
8
6
4
2
0
-2
-4
-6
-8
0
2
4
6
8
10
12
K=a
E(K) Along [100]
E(K) Along [110]
E(K) along [111]

Fig A3.5