PHYSICAL REVIEW B VOLUME 19, NUMBER 5 1 MARCH 1979

The magnetism of iron

J. Hubbard
IBM Research Laboratory, San Jose, California 95193
(Received 28 August 1978)

A type of theory capable of reconciling the localized- and itinerant-electron models of a ferromagnetic metal is discussed. This kind of theory contemplates a distribution of "exchange field" configurations which correspond very roughly to the spin configurations of the localized model. Computations involve thermal averages over these configurations, each configuration V having an effective energy $E(V)$. Starting from the band structure for ferromagnetic iron, the $E(V)$ have been estimated for certain configurations V. The results are reasonably consistent with the observed Curie temperature of iron, in spite of the presence of exchange fields ~1–2 eV, and give some suggestion of behavior characteristic of the Heisenberg model.

I. INTRODUCTION

The development of a satisfactory theory of ferromagnetic metals has been made difficult by the experimental data. Some data are readily interpretable in terms of a band-theory (itinerant-electron) model, other data in terms of a localized-electron model. For example, how in the localized model can one understand the non-half-integral atomic moments observed? Or how, in the itinerant model, explain a Curie temperature ~1000 °K for iron when calculations always give an exchange field ~1–2 eV?

These questions have, of course, been the subject of much debate over the years (see, for example, Herring[1]). Some progress in the right direction has been made by starting from the itinerant model and allowing approximately for spin-fluctuation effects,[2,3] but the relationship of these results to the localized picture remains vague. The experimental results suggest that one could usefully look for some sort of amalgam of the localized and itinerant models. One approach to such a theory is represented (within its limitations) by the work of Prange *et al.*,[4–7] which has much in common with the ideas presented here. An alternative way in which such an amalgam might be achieved is revealed by the older type of theory developed by Schrieffer, Evanson, and Wang[8–10] and by Cyrot.[11–13] In this paper we have followed the latter approach; the prime question studied is: Can the Schrieffer-Cyrot kind of theory give a reasonable account of the properties of a ferromagnetic metal such as iron?

The theories of Refs. 8–13 are necessarily based upon the functional-integral technique[14,15] for many-body problems, since this is the only known technique which gives the desired kind of result. However, the application of this technique is beset with ambiguities and alternative methods of formulation (see Appendix A). For example, the formulation of the method corresponding most closely to the approach of this paper is different from any used in Refs. 8–13; this new formulation is derived in Appendix A (it has also been independently derived by Prange and Korenman[7]). Thus, if the applicability of the method to iron is to be tested these ambiguities must be avoided or resolved. To this end we have in the main body of the paper made use of only the most general results [Eqs. (1)–(4) of Sec. III] obtained by functional-integral method. Remaining ambiguities have been resolved by an appeal to certain physical arguments and some parameters have been fixed by a study of the relationship of the method to the Hartree-Fock ferromagnetic-ground-state calculations. The rather general results obtained in this way have then been augmented by certain special calculations (see Secs. IV and V) to test how the method might work when applied to iron.

The results obtained in this way do, indeed, suggest that such an approach is of value. They provide an explanation of why the Curie temperature of iron is so low in spite of the largeness of the exchange fields (~1–2 eV). They give an indication of why iron seems in some experiments to behave very much like a Heisenberg model of localized spins. However, an attempt to reduce the results more precisely to a Heisenberg model along the lines of Cyrot's[11] cluster expansion suggestion did not work very well.

The general plan of this paper is as follows. In Sec. II we motivate the theory by a discussion of one of the serious problems facing the itinerant model, namely the low value of the Curie temperature T_C compared to the necessary exchange fields. A way out of this dilemma, suggested by the localized model, is considered and the resulting physical picture described. In Sec. III the manner in which this physical picture may be formalized using the functional-integral method is specified and its relationship to the Hartree-Fock ground-state calculations indicated. In Secs. IV and V we detail approximate calculations (based upon the ferromagnetic band structure) of the energy of an "impurity" in the ferromagnetic ground state of iron, the impurity being an iron atom with its moment reversed (in Sec. IV) or turned at an angle (in Sec. V) relative to the direction of magnetization. These calculations provide useful information concerning the energies $E(V)$ which appear in the formulation of Sec. III and suggest that this formulation is actually capable of resolving the T_C problem. Some conclusions are given in Sec. VI. In Appendix A the ambiguities of the functional-integral method are discussed and the variant closest to that required by the arguments of Sec. II is derived. In Appendix B certain technical details relating to the calculations of Sec. IV and V are described.

II. PHYSICAL PICTURE

The need for the kind of theory to be discussed (at least in the case of iron) may be illustrated by considering the problem of calculating the Curie temperature T_C within the framework of band theory (itinerant-electron theory). Self-consistent calculations of the band structure of ferromagnetic iron[16] give a very reasonable account of the ground state properties, e.g., the size of the magnetic moment. Inevitably they give exchange splittings $\Delta_{\mathrm{ex}} \sim 2$ eV between the energies of the up and down spin d-electron bands. If one now tries to extend this calculation to finite temperatures and determine at what temperature the magnetization disappears, one obtains an estimate T_C^{band} for the Curie temperature given by $k_B T_C^{\mathrm{band}} \sim \Delta_{\mathrm{ex}}$, i.e., $T_C^{\mathrm{band}} \sim 20\,000$ °K, since the only excited states entering the calculation are the Stoner excitations of electrons from the majority to the minority spin band. As the observed Curie temperature $T_C \sim 1000$ °K, one must conclude that there exist other more important excited states, that these other excitations have much lower energy and are capable of reducing the magnetic moment.

What is the nature of these excitations? They might be thought of as some sort of spin-wavelike collective mode; it is this thinking which underlies the work of Moriya *et al.*[2] and Klenin *et al.*[3] Another approach is suggested quite naturally by consideration of the localized electron model. In this model the magnetization is reduced as the temperature increases not by a reduction in the magnetic moments of the atoms (as in the case of the Stoner excitations), but by the appearance of excited states in which the atomic moments are no longer oriented parallel to each other, but are to some degree randomized in direction.

How would one describe such excitations in the itinerant model? One approach is exemplified by the work of Prange *et al.*[4–7] An alternative method, based upon the notion of the exchange field, will be described here. The total magnetic moment on an atom is a vector quantity $\vec{s}$. Furthermore, the exchange interaction is sufficiently localized in nature for one to think of the exchange field acting on the electrons of an atom to be mainly determined by the magnetic moment of that atom. Thus one would expect the exchange field at an atom with moment $\vec{s}$ to be given by $\vec{v} = J\vec{s}$ where J is some constant [the exchange field has in reality the character of a vector in spin space, see Appendix A or Eqs. (21)–(23)]. In the ground state all the atomic moments are parallel and the same exchange field exists at all atoms [as indicated schematically in Fig. 1(a)]. However, in an excited state in which the directions of the atomic moments are disordered the exchange field varies in direction from atom to atom as indicated in Fig. 1(b). This suggests that the low-energy excited states of the itinerant model are states in which the exchange field varies from atom to atom, and so are not easily describable in ordinary band theory, except in some special cases of high symmetry such as an antiferromagnetic arrangement.

One is led in this way to the following physical picture. At temperature $T = 0$ only the ground state is important, the exchange field is the same at all atoms and band theory calculations are good. At temperatures $\sim T_C$ many other excited states in which the exchange field varies from atom to atom are present.

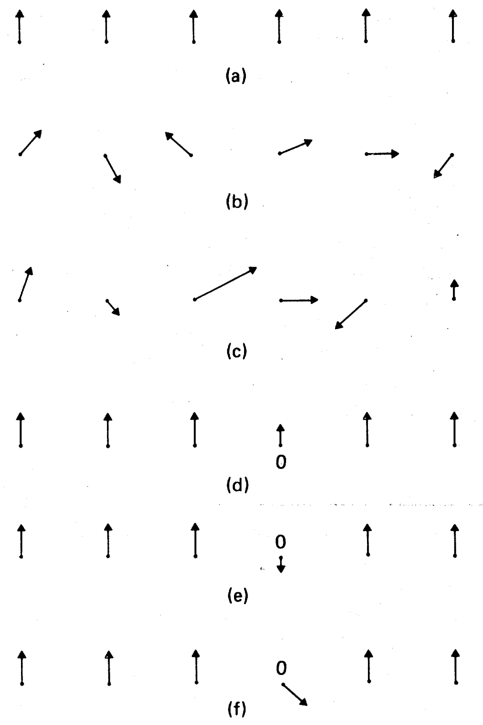

FIG. 1. Various exchange-field configurations (see text).

As the itinerant electrons move from atom to atom they are influenced by the variable exchange field in such a way that if the exchange field at an atom is $\vec{v}$ there will be a preponderance of electrons at that atom with spin in the direction $\vec{v}$; it is this preponderance which in turn generates the field $\vec{v}$ in a kind of selfconsistent fashion. One may think roughly of the localized model as giving a description not of the spins of electrons localized at the atoms, but rather of exchange fields localized at atoms. The electrons are itinerant, but are influenced in their motion by the localized exchange fields in a way which tends to make the latter self-maintaining. It is this physical picture which may be formalized in the kind of theory developed by Cyrot[11-13] and Schrieffer *et al.*,[8-10] to be discussed in Sec. III.

III. EXCHANGE FIELD DISTRIBUTION

We next discuss how the physical picture of Sec. II can be rendered into a computational scheme. One is contemplating a distribution of exchange fields corresponding roughly to the distribution of spin configurations of the localized model. The only method known to lead naturally from first principles to such a picture is the functional integral technique[14,15] for many-body problems, and it is this technique which was used in Refs. 7–13. As was pointed out in Sec. I, and is discussed further in Appendix A, the application of this method suffers from serious ambiguities. For this reason we will only make use of its most central results.

The results we shall require (see Refs. 8–13 and Appendix A for more details) are that one can write the partition function at temperature T approximately in the form

$$Z(T)=\sum_{\{V\}}\exp[-\beta E(V,T)]\ , \tag{1}$$

and that any electronic property X can be approximately written in the form

$$X(T)=Z^{-1}\sum_{\{V\}}X(V,T)\exp[-\beta E(V,T)]\ . \tag{2}$$

Here V describes (for more detail see below) some exchange field configuration, $\beta=1/k_BT$, T is the absolute temperature, k_B is Boltzmann's constant, $E(V,T)$ is a kind of energy associated with the configuration V, and $X(V,T)$ is the contribution to X associated with the configuration V; the sums (more strictly integrals) are over all configurations V. Furthermore, $E(V,T)$ has the form

$$E(V,T)=Q(V)+F(V,T)\ , \tag{3}$$

where $Q(V)$ is a quadratic function of the field V and $F(V,T)$ the thermodynamic potential (at temperature T) of a system of noninteracting electrons moving in the exchange field specified by V. $X(V,T)$ is just the value of the property X calculated for noninteracting electrons in the field V.

The ambiguities of the method center upon the nature of the exchange fields specified by V and the coefficients occurring in the quadratic $Q(V)$ of Eq. (3). We will make a choice which corresponds most closely to the physical picture of Sec. II. This choice differs in one way or another from any of these used in Refs. 8–13 and is discussed in Appendix A. For this particular choice, V specifies a set $\{\vec{v}_1,\vec{v}_2,\ldots\}$ of vector exchange fields, $\vec{v}_1$ at atom 1, $\vec{v}_2$ at atom 2, etc. (the $\vec{v}_i$ may be of any magnitude and direction). Further, $E(V)$ takes the form

$$E(V,T)=J^{-1}\sum_i\vec{v}_i^{\,2}+F(V,T)\ , \tag{4}$$

where J is a constant energy and $F(V,T)$ is the thermodynamic potential of noninteracting electrons moving in the atomic exchange fields $\vec{v}_i$ [the way in which a vector exchange field acts on electrons is specified at Eqs. (21)–(22)]. Thus, for example, the ground state of the ferromagnet corresponds to the configuration $V=\{-\vec{u},-\vec{u},-\vec{u},\ldots\}$, where $\vec{u}$ is a vector with the direction of the magnetization and magnitude equal to the exchange field in the ground state.

It may be seen that the formalism described above corresponds very closely to the physical picture of Sec. II. The configuration $V=\{\vec{v}_1,\vec{v}_2,\ldots\}$ corresponds to the state with atomic exchange fields $\vec{v}_1,\vec{v}_2,\ldots$ and therefore roughly to one of the spin configurations of the localized model. Any quantity X (e.g., the magnetic moment, an electron Green's function, etc.) is expressed as a thermal average over the exchange field configurations V, just as in the localized model it would be expressed as an average over spin configurations. However, the contribution $X(V)$ corresponding to a configuration is calculated for itinerant electrons in the field V. What the functional integral method has particularly provided is the prescription (4) for $E(V)$, the "energy" to be associated with the configuration V when forming the thermal averages.

If the theory is suitably formulated (see Appendix A) it bears a simple relationship to the Hartree-Fock ground state. If $T\to 0$ the sums in Eqs. (1) and (2) are dominated by the configuration $V_0=\{\vec{v}_1^{\,0},\vec{v}_2^{\,0},\ldots\}$ with the lowest energy $E(V)$. In fact, from Eq. (1) one sees that at $T=0$ the energy of the system is just $E(V_0)$ and the value of any quantity X is just $X(V_0)$. Thus one would expect V_0 to correspond to the exchange field in the ground state. Since $E(V)$ is a minimum at $V=V_0$, one has

$$\left.\frac{\partial E(V)}{\partial\vec{v}_i}\right|_{V=V_0}=0\quad\text{all } i\ , \tag{5}$$

which gives, using Eq. (4),

$$\vec{v}_i^{\,0} = -\tfrac{1}{2}J\,\frac{\partial F(V)}{\partial \vec{v}_i}\bigg|_{V=V_0} = -J\vec{m}_i^{\,0}\,, \tag{6}$$

where $\vec{m}_i^{\,0}$ is the spin moment at atom i calculated (at $T=0$) for electrons moving in the field V_0. Equation (6) is just equivalent to the Hartree-Fock equations if the parameter J is identified as that giving the relation between the exchange field at an atom and the moment of that atom. Furthermore, $E(V_0)$ coincides with the total binding energy calculated according to Hartree-Fock theory; $F(V_0)$ is the total energy of the electrons in the field V_0 and the first term of Eq. (4) allows for the double counting of the exchange energy in $F(V_0)$.

Of course, Eq. (6) may have many solutions and one must pick the one giving the lowest $E(V_0)$ to obtain the ground state. In the case of a ferromagnet we would expect this to correspond to

$$\vec{v}_i^{\,0} = -\vec{u}\,,\quad \vec{m}_i^{\,0} = \vec{m}\quad \text{for all } i \text{ with } \vec{u} = J\vec{m}\,, \tag{7}$$

i.e., the same exchange field $-\vec{u}$ and the same moment $\vec{m}$ at all atoms. Equation (6) will determine the magnitude of $\vec{u}$ and $\vec{m}$, but not their direction (the magnetization may be in any direction since no effects giving rise to anisotropy in spin space have been considered). One sees that the parameter J may be obtained independently of the ambiguous first-principles theory of Appendix A from a knowledge of the Hartree-Fock ground-state solution. The latter gives both the strength of the exchange field and the moment per atom whence J may be obtained using Eq. (7). From the calculations of Tawil and Callaway[16] for iron we estimated a value $J=0.85$ eV in this way.

It may be noted that the theory formulated via Eqs. (1)–(4) is actually more general than that contemplated in Sec. II. In Sec. II we considered only the possibility that the atomic exchange field might be turned at an angle to the direction of magnetization (as do Prange *et al.*[4–7]). However, the formulation described above also admits the possibility that the exchange field might vary in magnitude as well as direction from atom to atom since the $\vec{v}_i$ may vary in magnitude as well as direction [as indicated schematically in Fig. 1(c)]. This circumstance enables one to investigate to some extent how closely the behavior of the system does resemble that of a localized Heisenberg model in which the spins only rotate without change of magnitude (see Sec. V).

It has been argued in Sec. II that a theory of the kind reviewed above might provide an escape from the difficulty with the magnitude of T_C in the itinerant theory. In the rest of this paper we consider whether it might actually work when applied to the case of iron. The crucial question here concerns the magnitudes of the energies $E(V)$ for configurations V with magnetic moments $M(V)$ which are small compared to that of the ground state. If the theory is to account for the observed T_C, then the energy differences $\Delta E(V)=E(V)-E(V_0)$ between these configurations V and the ground state configuration V_0 must be $\sim$0.2 eV per reversed spin in V (relative to V_0), in spite of the fact that the exchange fields themselves have the order of magnitude $\sim$1 eV. We shall, in fact, obtain some evidence that the relevant ΔE are of this order of magnitude.

IV. ENERGY OF SPIN REVERSAL

In this and Sec. V we shall address the question posed at the end of Sec. III by describing some calculations which yield information concerning the magnitudes of the energy differences ΔE in iron. The general problem of calculating $E(V)$ from Eq. (4) is a very difficult one since it involves estimation of the thermodynamic potential $F(V)$ of electrons moving in the disordered exchange field specified by V. Cyrot[12,13] investigated the problem by making a cluster expansion of F and also by applying the coherent potential method (see also Liu[17]). Prange *et al.*[4–7] base their calculations on a perturbation expansion for F appropriate when the angle between neighboring $\vec{v}_i, \vec{v}_j$ is small. We have preferred to follow the approach of Schrieffer *et al.*[9] and obtain information about the $\Delta E(V)$ by the consideration of more precise calculations which are possible for certain special configurations V. In particular, in this and Sec. V we study the case in which the configuration V differs from the ferromagnetic ground-state configuration V_0 in only one respect, namely that the exchange field at a single atom has been changed from its ground-state value. In this case one is dealing essentially with the problem of an "impurity" atom in the ferromagnet and the change ΔF may be expressed relatively simply in terms of the (assumed known) ferromagnetic band structure.

Suppose the magnetization is in the z direction and that the electron spins are quantized in this direction so that the majority spins have spin $\sigma=1$, the minority spin $\sigma=-1$. The corresponding ground-state configuration V_0 is given by

$$V_0\colon\ \vec{v}_i = -u\hat{z}\quad \text{for all } i\,, \tag{8}$$

where u is the strength of the exchange field in the ground state and $\hat{z}$ a unit vector in the z direction. In this section we shall consider the change in energy $\Delta E(V_1)$ on going to the configuration V_1 [shown schematically in Figs. 1(d) and (e)] in which the exchange field at one atom, $i=0$, is changed but remains parallel or antiparallel to the direction of magnetization,

$$V_1\colon\ \vec{v}_i = -u\hat{z}\quad \text{if } i \neq 0,\quad \vec{v}_0 = (\mathrm{v}-u)\hat{z}\,. \tag{9}$$

The change in the exchange field at atom 0 is $\mathrm{v}\hat{z}$;

$v < u$ represents a reduced field [Fig. 1(d)] and $v > u$ a reversed field [Fig. 1(e)] at site 0.

To estimate $\Delta E(V_1)$ for iron we will make various simplifying assumptions which we hope will not invalidate the conclusions. We will study only the *d* band, neglecting effects of hybridization with the *s* band. Let us denote by $\phi_{is\sigma}$ the *d*-band Wannier functions of the ferromagnetic band structure, where $s = 1, 2, \ldots, 5$ labels the five subbands and $\sigma = \pm 1$ the spin. We will assume that the $\phi_{is\sigma}$ are so localized that the exchange field $\vec{\mathrm{v}}_i$ acts only upon the $\phi_{is\sigma}$ (i.e., not on the $\phi_{js\sigma}$ with $j \neq i$) and that it acts equally on all the $\phi_{is\sigma}$ with different *s* and oppositely on $\phi_{is\sigma}$ with opposite σ.

The exchange field in the configuration V_0 has translational symmetry and this case can be completely solved by ordinary band theory. The result is, of course, the ferromagnetic band structure with energy levels $\epsilon_{\vec{\mathrm{k}}s\sigma}$ ($\vec{\mathrm{k}}$ is the Bloch wave vector) and the corresponding Wannier functions $\phi_{is\sigma}$.

The configuration V_1 differs only from V_0 in that there is an additional impurity exchange field v at site 0. The Hamiltonian describing the electron motion in this case can therefore be written

$$H = \sum_{\vec{\mathrm{k}}s\sigma} \epsilon_{\vec{\mathrm{k}}s\sigma} c^{\dagger}_{\vec{\mathrm{k}}s\sigma} c_{\vec{\mathrm{k}}s\sigma} + \mathrm{v} \sum_{s\sigma} \sigma n_{0s\sigma} , \tag{10}$$

where the $c_{\vec{\mathrm{k}}s\sigma}$ are the destruction operators for the ferromagnetic band states, the first term describes ferromagnetic band structure, and $n_{is\sigma} = c^{\dagger}_{is\sigma} c_{is\sigma}$, where $c_{is\sigma}$ is the destruction operator for an electron in the Wannier orbital $\phi_{is\sigma}$,

$$c_{is\sigma} = N^{-1/2} \sum_{\vec{\mathrm{k}}} c_{\vec{\mathrm{k}}s\sigma} \exp(i\vec{\mathrm{k}} \cdot \vec{\mathrm{R}}_i) , \tag{11}$$

where $\vec{\mathrm{R}}_i$ is the position of the atom *i* and *N* the number of atoms; the second term of Eq. (10) describes the effect of the impurity field at atom 0.

The change in the thermodynamic potential *F* of the electrons due to the impurity term in Eq. (10) can be calculated in a standard fashion (see Appendix B) and the result can be written (at $T = 0$ which will suffice for the present purpose since $k_B T_C \ll$ *d*-electron bandwidth),

$$\Delta F[V_1] = \int_{-\infty}^{\mu} d\omega \frac{1}{\pi} \sum_{s\sigma} \delta_{s\sigma}(\omega) , \tag{12}$$

where μ is the Fermi energy. The $\delta_{s\sigma}(\omega)$ are "phase shifts" due to the impurity potential for electrons of energy ω in the $s\sigma$ subband, given by

$$\delta_{s\sigma}(\omega) = \arctan \frac{\sigma \pi \mathrm{v} \rho_{s\sigma}(\omega)}{1 - \sigma \mathrm{v} G'_{s\sigma}{}'(\omega)} , \tag{13}$$

(the branch between 0 and π must be taken for $\sigma = 1$, between 0 and $-\pi$ for $\sigma = -1$), where

$$\rho_{s\sigma}(\omega) = N^{-1} \sum_{\vec{\mathrm{k}}} \delta(\omega - \epsilon_{\vec{\mathrm{k}}s\sigma}) \tag{14}$$

is the density of states per atom of the $s\sigma$ subband and

$$G'_{s\sigma}(\omega) = \mathrm{P} \int \frac{\rho_{s\sigma}(\omega')\, d\omega'}{\omega - \omega'} , \tag{15}$$

where P indicates the principal-value integral [so $G'_{s\sigma}(\omega) + i\pi\rho_{s\sigma}(\omega)$ is the single-site retarded Green's function for the $s\sigma$ subband at energy ω, see Appendix B].

The formulas (12)–(15) show that ΔF can be obtained simply from a knowledge of the densities of states $\rho_{s\sigma}(\omega)$, so these quantities represent all the information required concerning the ferromagnetic band structure for the present purpose. Inspection of the total densities of states for ferromagnetic iron calculated by Tawil and Callaway[16] shows that to a good approximation the $\sigma=1$ and $\sigma=-1$ bands are rigidly translated in energy relative to each other, so it is possible to write

$$\rho_{s\sigma}(\omega) \simeq \rho_s(\omega + \sigma u) , \tag{16}$$

where *u* is the same exchange field that appears in Eq. (8). Unfortunately we did not have available the $\rho_s(\omega)$ for the individual subbands and so have made the approximation

$$\rho_s(\omega) = \tfrac{1}{5}\rho(\omega) , \tag{17}$$

where $\rho(\omega)$ is the total *d*-band density of states (for one spin direction); it is desirable that these calculations be repeated with the proper $\rho_s(\omega)$.

$\rho(\omega)$ was estimated from the densities of state for the up and down spin directions given in Ref. 16 by subtracting out an estimate of the *s*-band contribution to the density of states. At the same time we obtained an estimate $u=0.95$ eV for the exchange field and $\mu=4.06$ eV measured relative to the bottom of the *d* bands (before they were shifted up and down by the potential *u*), which correspond to 7.36 electrons in the *d* band and a moment of 2.22 Bohr magnetons per atom.

The total change in energy $\Delta E(V_1)$ is given, according to Eq. (4), by

$$\Delta E(V_1) = J^{-1}[(\mathrm{v}-u)^2 - u^2] + \Delta F , \tag{18}$$

with ΔF given by Eq. (12) and $J=0.85$ eV estimated as described in Sec. III. $\Delta E(V_1)$ was evaluated using Eqs. (12)–(18) and the $\rho(\omega)$ obtained as described above. The result is plotted as a function of v in Fig. 2. Of course there is a minimum at v=0, but what is of more interest is the appearance of a second minimum at v=2.35 eV corresponding to more than a complete reversal of the exchange field. The corresponding change in the magnetic moment may be estimated since one may show (see Appendix B) that the change ΔM in the total magnetic moment due to the impurity term in Eq. (10) is given by

$$\Delta M = -\frac{1}{\pi}\sum_{s\sigma} \sigma\delta_{s\sigma}(\mu) \ . \qquad (19)$$

At v=2.35 eV one finds $\Delta M = -4.65$ Bohr magnetons, so at this minimum the change in M corresponds almost exactly to the reversal of the moment of one atom.

The energy change $\Delta E(V_1)$ at the minimum v=2.35 eV is $\Delta E = 0.194$ eV, very small in spite of the large exchange fields involved. One has, in fact, found a configuration in which the moment of one atom is reversed with an excitation energy of order of magnitude 0.1 eV as was required according to the discussion at the end of Sec. III. Indeed, in the Heisenberg model one has $k_B T_C \simeq \frac{1}{3}\Omega$, where Ω is the energy required to reverse one spin in the ferromagnetic state (for the case spin=1, roughly corresponding to iron), so a value $\Omega = 0.194$ eV would give $T_C \simeq 700$ K, a surprisingly good result in view of the many approximations.

One may note that the second minimum in Fig. 2 occurs at v=2.35 eV, rather greater than $2u = 1.9$ eV, and that the peak in Fig. 2 is by no means symmetrically disposed between the two minima. For these reasons it was not found possible to make any reasonable fit of the curve of Fig. 2 to the sort of cluster expansion result suggested by Cyrot [Ref. 11, Eq. (11)].

V. ENERGY OF SPIN ROTATION

In this section we consider a slightly more general case than that of Sec. IV, namely one in which the exchange field at a single site is rotated away from the ferromagnetic direction as well as changed in magnitude. In other words, we consider configurations of the type shown schematically in Fig. 1(f). In this configuration the exchange fields have the form

$$V_2\text{: } \vec{v}_i = -u\hat{z} \ \text{ for } i \neq 0, \ \vec{v}_0 = \vec{v} - u\hat{z} \ , \qquad (20)$$

where one can assume without loss of generality that $\vec{v}$ is an arbitrary vector in the x-z plane: $\vec{v} = (v_x, 0, v_z)$.

One has again an impurity problem to deal with in calculating ΔF, the impurity being the additional exchange field $\vec{v}$ at site 0. In Sec. IV the impurity field was in the z direction and gave rise to the last term in Eq. (10). In the present case this term is replaced by

$$2\vec{v}\cdot\vec{S}_0 \qquad (21)$$

representing the interaction of the electrons with the additional field at site 0, $\vec{S}_i$ being the total electron spin operator at site i given by

$$S_i^\alpha = \frac{1}{2}\sum_s \sum_{\sigma\sigma'} \Lambda^\alpha_{\sigma\sigma'} c^\dagger_{is\sigma} c_{is\sigma'} \ , \quad \alpha = x,y,z \ , \qquad (22)$$

where the s sum is over the five d subbands, the σ, σ' sums over ± 1 and the Λ^α are the Pauli matrices

$$\Lambda^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \Lambda^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \Lambda^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} . \qquad (23)$$

$\Delta F(V_2)$ may now be calculated much as $\Delta F(V_1)$ was (see Appendix B), the previous result (12) being generalized to

$$\Delta F(V_2) = \frac{1}{\pi}\int_{-\infty}^{\mu} d\omega \sum_s \mathrm{tr}\,\underline{\delta}_s(\omega) \ , \qquad (24)$$

where tr means the trace over the $\underline{\delta}_s(\omega)$ which are now 2×2 matrices in spin space defined by

$$\underline{\delta}_s(\omega) = \mathrm{Im}\ln[1 - \underline{V}\,\underline{G}_s(\omega)] \ , \qquad (25)$$

where Im means imaginary part,

$$\underline{V} = \begin{pmatrix} v_z & v_x \\ v_x & -v_z \end{pmatrix} \qquad (26)$$

and

$$\underline{G}_s(\omega) = \begin{pmatrix} G'_{s\uparrow} + i\pi\rho_{s\uparrow} & 0 \\ 0 & G'_{s\downarrow} + i\pi\rho_{s\downarrow} \end{pmatrix} . \qquad (27)$$

$G'_{s\sigma}$, $\rho_{s\sigma}$ being defined at Eqs. (14) and (15). $\Delta E(V_2)$ is given by

$$\Delta E(V_2) = J^{-1}[(\vec{v} - u\hat{z})^2 - u^2] + \Delta F(V_2) \ . \qquad (28)$$

$\Delta E(V_2)$ was calculated as a function of (v_x, v_z) from the formulas (24)–(28) using exactly the same assumptions concerning the form of the $\rho_{s\sigma}$ as in Sec. IV. In Fig. 3 a contour plot of $\Delta E(V_2)$ against $\vec{v}$ is given [$\Delta E(V_2)$ is symmetrical under the reflection $v_x \rightarrow -v_x$].

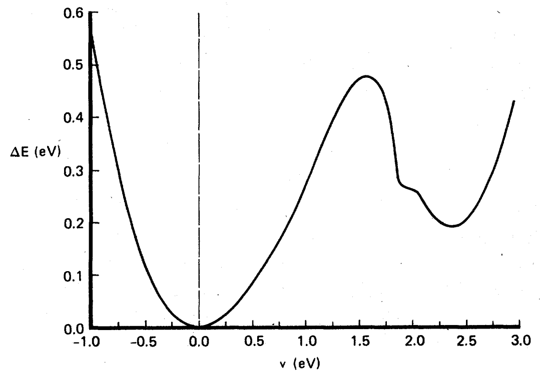

FIG. 2. The excitation energy $\Delta E(V_1)$ as a function of the change v in the exchange field at one site (see Sec. IV).

Figure 3 reveals the presence of a ring shaped valley in the $\Delta E(V_2)$ surface. The two minima of Fig. 2 correspond to the points where the $v_x=0$ section of this surface intersects the floor of the valley. Figure 3 indicates that the lowest-energy excitations correspond to configurations V in which the exchange field is rotated away from the ferromagnetic direction without substantial change in magnitude, a result giving some support to the view that the important configurations are those corresponding roughly to the Heisenberg picture. This result supports the method of calculation of Prange *et al.*[4-7] (at least for iron) in the sense that it shows the most important excitations to be spin rotational in nature; the question of whether the angles between neighboring spins remain small is left open, however.

To pursue this point further, we have plotted in Fig. 3 the curve *ABO* marking the floor of the valley. It will be seen that it is almost a perfect circle centered on the point C at which $\vec{v}=(0,0,1.2)$ eV. It seems probable that if the change $\Delta\vec{M}(V_2)$ in the magnetic moment were calculated one would find that this circle corresponds to the rotation of the magnetic moment of a single atom (we have so far only calculated $\Delta\vec{M}$ for the case $v_x=0$).

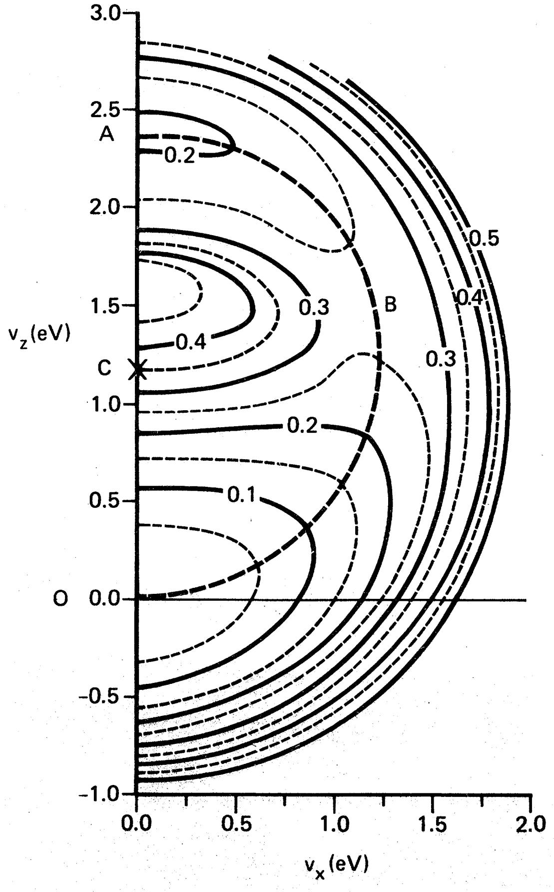

FIG. 3. Contour plot of the excitation energy $\Delta E(V_2)$ (in eV) against (v_x, v_z), the components of the change in the exchange field at one site; the broken line *OBA* marks the "floor of the valley" (see Sec. V).

In the Heisenberg model the change in energy on rotating a single spin out of the ferromagnetic direction has the form

$$\Delta E = J_1 \sin^2(\phi/2) , \tag{29}$$

where J_1 is some combination of the spin coupling parameters and ϕ the angle of rotation. In Fig. 4 we have, for comparison, plotted the energy $\Delta E(V_2)$ along the line *OBA* of Fig. 3 as a function of the angle ϕ of rotation about C (from *CO*). This curve does not have exactly the form (29), but bears some resemblance to it [a curve of the form (29) with J_1 chosen to have the same area under it has been plotted in Fig. 4 for comparison]. The use of J_1 obtained in this manner would give $T_C \sim 1200$ °K.

VI. CONCLUSIONS

On the basis of the calculations of Secs. IV and V, limited in scope though they may be, we would like to draw some tentative conclusions. These calculations seem clearly to open up the possibility that the type of theory described in Secs. II and III can actually explain the coexistence of a low T_C and rather large exchange fields and thus resolve a long standing problem. They imply that two energy scales are operative in iron, one of the order of electron volts which is characteristic of the itinerant behavior (e.g., the bandwidth and the exchange fields), and another of the order of one tenth of an electron volt characteristic of the "localized" behavior [e.g., $k_B T_C$, the $\Delta E(V)$]. The theory of Refs. 8–13 and Sec. III is seen to provide a rather neat synthesis of the itinerant and localized behavior; the evaluation of the sums in Eqs. (1) and (2) is analogous to the calculation of thermal averages over the spin configurations of a localized model with Boltzmann factors involving the "localized" energies $\Delta E(V)$; but the quantities $X(V)$ in Eq. (2) and $F(V)$ in Eqs. (3) and (4) must be evaluated according to itinerant electron theory.

Finally it should be remarked that the calculations of Sec. V gave a strong indication of behavior characteristic of the Heisenberg model in that the most important excited configurations V were found to be those corresponding to the rotation of the atomic moment rather than a change in magnitude of the moment.

APPENDIX A: FUNCTIONAL-INTEGRAL DERIVATION

The derivation of the kind of results represented by Eqs. (1)–(4) has been discussed at length in Refs.

2–7, so we shall only consider here some aspects which are most relevant to the arguments of this paper. The results always follow from an identity of the form[2–9]

$$\int \prod_{i\alpha} [Dv_i^\alpha(t)] \exp\left[-K \sum_{i\alpha} \int_0^\beta [v_i^\alpha(t)]^2\, dt\right] \mathrm{Tr}\exp_+\left[-\int_0^\beta H_0(t)\, dt - \sum_{i\alpha} \int_0^\beta v_i^\alpha(t)\, X_i^\alpha(t)\, dt\right]$$

$$\propto \mathrm{Tr}\exp\left[-\beta H_0 + \beta (4K)^{-1} \sum_{i\alpha} X_i^\alpha X_i^\alpha\right] , \qquad \text{(A1)}$$

where i labels atoms, $v_i^\alpha(t)$ is some "field" at site i defined for t on $(0, \beta)$ (α labels the different components), $Dv_i^\alpha(t)$ indicates a functional integration over the field component $v_i^\alpha(t)$, Tr means the quantum mechanical trace over the Hilbert space of the system, $\exp_+$ means the time-ordered exponential, $H_0 = \mathcal{H} - \mu N_e$ where $\mathcal{H}$ is the Hamiltonian describing the band motion of the electrons, N_e is the electron number operator, and μ the Fermi energy, and the X_i^α are one electron operators acting on the electrons at site i (bilinear combinations of the $c_{is\sigma}^\dagger$ and $c_{is\sigma}$ of Sec. IV). This identity is applied by choosing K and the X_i^α so that the last term in the exponent on the right-hand side represents the electron interaction, which makes the right-hand side of Eq. (A1) just equal to the grand partition function; the left-hand side then gives a representation of the partition function as a functional integral. The usual first approximation is to neglect the time-fluctuating part of the fields $v_i^\alpha(t)$ in the functional integral and write it as an ordinary integral,

$$Z \propto \int \prod_{i\alpha} (dv_i^\alpha) \exp\left[-\beta K \sum_{i\alpha} (v_i^\alpha)^2\right]$$

$$\times \mathrm{Tr}\exp\left[-\beta H_0 - \beta \sum_{i\alpha} v_i^\alpha X_i^\alpha\right] . \qquad \text{(A2)}$$

In simpler cases[9] this approximation involves the neglect of certain collective behavior, but in view of the ambiguities discussed below we may suspect it of having more serious implications in this case.

The ambiguity of the method arises from the fact that it may be possible to resolve the electron interaction into a quadratic form $(4K)^{-1} \sum_{i\alpha} X_i^\alpha X_i^\alpha$ in more than one way. Equation (A1) remains true whatever decomposition is used, but after the approximation (A2) has been made one may obtain different results from different decompositions. For example, in the case of the narrow energy-band model with one orbital per atom of each spin and the Hamiltonian

$$H' = \mathcal{H} + U \sum_i n_{i\uparrow} n_{i\downarrow} , \qquad \text{(A3)}$$

the following decompositions of the interaction

$$U n_{i\uparrow} n_{i\downarrow} = \tfrac{1}{2} U n_i - 2U (S_i^z)^2 \qquad \text{(A4a)}$$

$$= \tfrac{1}{4} U n_i^2 - U (S_i^z)^2 \qquad \text{(A4b)}$$

$$= \tfrac{1}{4} U n_i^2 - \tfrac{1}{3} U \vec{S}_i^2 \qquad \text{(A4c)}$$

are some of the possible alternatives, [Eq. (A4a) used in Refs. 9 and 11, Eq. (A4b) in Ref. 18, and Eq. (A4c) in Refs. 12 and 13], where $n_i = n_{i\uparrow} + n_{i\downarrow}, S_i^z = \frac{1}{2}(n_{i\uparrow} - n_{i\downarrow})$ and $\vec{S}_i$ is the total spin of atom i When Eq. (A4a) is used the field v_i has only one component, when Eq. (A4c) is used the field v_i is a vector $\vec{v}_i$ (attending only to the exchange part $U\vec{S}_i^2$); one has in these two cases

$$v_i \text{ scalar}, \quad X_i = 2S_i^z, \quad K = 1/2U , \qquad \text{(A5a)}$$

$$\vec{v}_i \text{ vector}, \quad \vec{X}_i = 2\vec{S}_i, \quad K = 3/U . \qquad \text{(A5b)}$$

The result (A2) is essentially of the form used in Sec. III since the Tr exp ... factor is just $e^{-\beta F}$ where F is the thermodynamic potential of the band electrons moving in the field $\sum_{i\alpha} v_i^\alpha X_i^\alpha$. However, the form (A5a) does not correspond to the physical picture of Sec. II since the field v_i is now a scalar and the rotational symmetry (in spin space) is lost. The form (A5b) is suitable in that respect, but has the defect that the procedure leading to Eq. (6) does not give the Hartree-Fock equations appropriate to the Hamiltonian (A3) (one obtains equations of the same form but with a coefficient $\frac{1}{3} U$ where one should have had U).

Thus none of the schemes so far used would, when applied to Eq. (A3), give a result of the kind looked for in Sec. II. Nevertheless, one can exploit the ambiguity to obtain a formulation of the required kind for the Hamiltonian (A3). To see this we introduce yet another decomposition of the interaction. (A4b) is derived by quantizing the electron spins in the z direction; however, one could equally well quantize them in the direction of the arbitrary unit vector $\vec{e}_i$ and obtain the identity

$$U n_{i\uparrow} n_{i\downarrow} = \tfrac{1}{4} U n_i^2 - U (\vec{e}_i \cdot \vec{S}_i)^2 . \qquad \text{(A6)}$$

Using this decomposition one would obtain from Eq. (A2) [omitting for simplicity the nonexchange term, the first term of Eq. (A6), which leads to the nonexchange part of the Hartree-Fock field],

$$Z \propto \int \prod_i dv_i \exp\left(-\beta K \sum_i v_i^2\right) \times \mathrm{Tr} \exp\left(-\beta H_0 - \beta \sum_i 2 v_i \vec{e}_i \cdot \vec{S}_i\right) . \quad (A7)$$

This form does not have rotational symmetry because the $(\vec{e}_i)$ have specified directions. However, since Eq. (A7) is supposed to hold for arbitrary $(\vec{e}_i)$, one could restore the symmetry by averaging Eq. (A7) over all directions for each $\vec{e}_i$. When this is done one obtains, writing $\vec{v}_i = v_i \vec{e}_i$,

$$Z \propto \int \prod_i d\vec{v}_i \exp\left(-\beta K \sum_i \vec{v}_i^2\right) \times \mathrm{Tr} \exp\left(-\beta H_0 - \beta \sum_i 2\vec{v}_i \cdot \vec{S}_i\right) , \quad (A8)$$

where one now has $K = 1/U$. This form does have a vector field $\vec{v}_i$ and does yield the Hartree-Fock equations by the procedure leading to Eq. (6). The same formula has been obtained by Prange and Korenman[7]; they make the further approximation of dropping the integration over the lengths of the $\vec{v}_i$, which they hold fixed, allowing only angular integration over the $\vec{v}_i$. The degree of ambiguity present may be seen by recognizing that the form (A8) is the same as that obtained from Eq. (A5b) except for the coefficient K.

Let us summarize some of the relevant results (for the theory of Sec. III) following from the above discussion: (a) in all cases Eq. (A2) has the form represented by Eq. (1) and (3) [and Eq. (2) follows easily]; (b) amongst the possibilities are those with rotational symmetry in which the field $\vec{v}_i$ is a vector and $E(V)$ has the form (4); (c) amongst the latter possibilities there exist some which lead to the Hartree-Fock result by the procedure described in Sec. III. The assumptions of Sec. III may thus be realized for the Hamiltonian (A3) in a suitable formulation of the method. It will be seen, however, why we wished to make minimal use of the first-principles theory, and preferred, for example, to determine the parameter J (or K in the above) by the procedure of Sec. III.

In the case of iron one is dealing with a d band and the Hamiltonian does not have the simple form (A3). What we did in practice was simply generalize the above results to this case by interpreting $\vec{S}_i$ as the total spin of an iron atom. This corresponds to assuming that the exchange field acts equally on all the d-electron states, i.e., is independent of the azimuthal component of the orbital momentum. The most general form for the exchange field could be written

$$\sum_\alpha v_i^\alpha X_i^\alpha = \sum_\alpha \sum_{ss'} \sum_{\sigma\sigma'} v_{ss'}^\alpha \Lambda_{\sigma\sigma'}^\alpha c_{is\sigma}^\dagger c_{is'\sigma'} \quad (A9)$$

in the notation of Secs. IV and V, involving the field

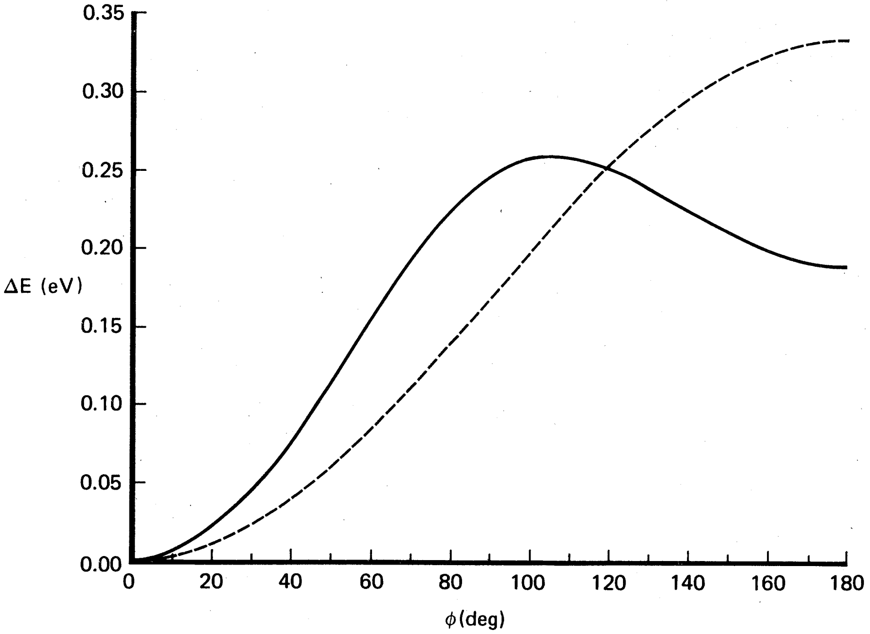

FIG. 4. The excitation energy $\Delta E(V_2)$ along the line OBA of Fig. 3 plotted as a function of the angle of rotation about C from CO (solid line); the broken line is a fit corresponding to the Heisenberg model (see Sec. V).

$v_{ss'}^{\alpha}$ with 75 independent parameters. The assumption that the action of the exchange field is independent of the spacial state is equivalent to taking

$$v_{ss'}^{\alpha}=\delta_{ss'}v^{\alpha} \tag{A10}$$

in which case Eq. (A9) reduces to $2\vec{v}_i\cdot\vec{S}_i$. We would expect that this assumption would not lead to large errors, but have little evidence on the point. It should be noted, however, that this assumption is consistent with the observation that the two spin bands calculated by Tawil and Callaway[10] are almost rigidly translated in energy relative to each other.

APPENDIX B: CALCULATION OF ΔF

In this appendix we briefly sketch the derivation of the results used in Secs. IV and V. The analysis is based upon that given in Ref. 5. We want to calculate the thermodynamic potential defined by

$$-\beta F=\ln \operatorname{Tr}\exp[-\beta(H-\mu N_e)]\ , \tag{B1}$$

where H' is the Hamiltonian (10). To this end we introduce the "unperturbed" Green functions $G_{s\sigma}^{ij}(z)$ between atoms i, j,

$$G_{s\sigma}^{ij}(z)=N^{-1}\sum_{\vec{k}}\frac{1}{z-\epsilon_{\vec{k}s\sigma}}\exp[i\vec{k}\cdot(\vec{R}_i-\vec{R}_j)] \tag{B2}$$

for the ferromagnetic band structure $\epsilon_{\vec{k}s\sigma}$, where the sum is over the Brillouin zone and N is the number of atoms. We may also introduce the corresponding perturbed Green's functions $g_{s\sigma}^{ij}(z)$ for the Hamiltonian (10) [a single $s\sigma$ label suffices since the impurity term in Eq. (10) does not mix the different subbands] and easily show[5] that

$$\begin{aligned} g_{s\sigma}^{ij}(z)&=G_{s\sigma}^{ij}(z)+G_{s\sigma}^{i0}(z)\sigma\mathrm{v}\\ &\quad\times[1-\sigma\mathrm{v}G_{s\sigma}(z)]^{-1}G_{s\sigma}^{0j}(z)\ , \end{aligned} \tag{B3}$$

where

$$\begin{aligned} G_{s\sigma}(z)&\equiv G_{s\sigma}^{00}(z)\\ &=N^{-1}\sum_{k}\frac{1}{z-\epsilon_{\vec{k}s\sigma}}=\int\frac{\rho_{s\sigma}(\omega)\,d\omega}{z-\omega}\ , \end{aligned} \tag{B4}$$

[$\rho_{s\sigma}$ defined at Eq. (14)].

Now, differentiating Eq. (B1) with respect to v [using Eq. (10)] one has[5]

$$\frac{\partial F}{\partial \mathrm{v}}=\sum_{s\sigma}\sigma\langle n_{0s\sigma}\rangle=i\beta^{-1}\sum_{s\sigma}\sum_{\nu}\sigma g_{s\sigma}^{00}(\omega_\nu) \tag{B5}$$

where the ν sum is over all ω_ν of the form $\omega_\nu=(i\pi\nu/\beta)+\mu$, $\nu=\pm1,\ \pm3,\ \pm5,\ \cdots$ Substituting Eq. (B3) into Eq. (B5) we have

$$\frac{\partial F}{\partial \mathrm{v}}=i\beta^{-1}\sum_{s\sigma}\sum_{\nu}\sigma G_{s\sigma}(\omega_\nu)[1-\sigma\mathrm{v}G_{s\sigma}(\omega_\nu)]^{-1}\ , \tag{B6}$$

which may be integrated at once to give

$$\Delta F=F-F_0=-i\beta^{-1}\sum_{s\sigma}\sum_{\nu}\ln[1-\sigma\mathrm{v}G_{s\sigma}(\omega_\nu)]\ , \tag{B7}$$

where F_0 is the thermodynamic potential at $\mathrm{v}=0$, i.e., that of the ferromagnetic ground state.

Transforming the ν sum into a contour integral in the usual way and deforming the contour to surround the real axis, Eq. (B7) gives

$$\begin{aligned} \Delta F=&-\sum_{s\sigma}\frac{1}{\pi}\int d\omega\,f(\omega)\\ &\times\operatorname{Im}\ln[1-\sigma\mathrm{v}G_{s\sigma}(\omega-i0^+)]\ , \end{aligned} \tag{B8}$$

where $f(\omega)$ is the Fermi-Dirac distribution function. From Eq. (B4) one has

$$G_{s\sigma}(\omega-i0^+)=G'_{s\sigma}(\omega)+i\pi\rho_{s\sigma}(\omega) \tag{B9}$$

using the definition (15). Substituting Eq. (B9) into Eq. (B8), taking the imaginary part and letting $T\to0$ so that $f(\omega)=1$ if $\omega<\mu$ and $f(\omega)=0$ if $\omega>\mu$, one obtains Eqs. (12) and (13).

The total magnetic moment (in the z direction) of the perturbed system is given by

$$M=\sum_{is\sigma}\sigma\langle n_{is\sigma}\rangle=i\beta^{-1}\sum_{is\sigma}\sum_{\nu}\sigma g_{s\sigma}^{ii}(\omega_\nu)\ . \tag{B10}$$

Substituting for $g_{s\sigma}^{ii}$ from Eq. (B3), one has for the change in the moment due to the perturbation

$$\begin{aligned} \Delta M=&\ i\beta^{-1}\sum_{s\sigma}\sum_{\nu}\mathrm{v}[1-\sigma\mathrm{v}G_{s\sigma}(\omega_\nu)]^{-1}\\ &\times\sum_{i}G_{s\sigma}^{i0}(\omega_\nu)G_{s\sigma}^{0i}(\omega_\nu)\ . \end{aligned} \tag{B11}$$

From Eqs. (B2) and (B4) we have

$$\sum_{i}G_{s\sigma}^{i0}(z)G_{s\sigma}^{0i}(z)=\frac{-\partial G_{s\sigma}(z)}{\partial z} \tag{B12}$$

so Eq. (B11) reduces to

$$\begin{aligned} \Delta M&=i\beta^{-1}\sum_{s\sigma}\sum_{\nu}\sigma\frac{\partial\{\ln[1-\sigma\mathrm{v}G_{s\sigma}(\omega_\nu)]\}}{\partial\omega_\nu}\\ &=\sum_{s\sigma}\sigma\frac{1}{\pi}\int d\omega\,f(\omega)\,\partial\\ &\qquad\times\{\operatorname{Im}\ln[1-\sigma\mathrm{v}G_{s\sigma}(\omega-i0^+)]\}/\partial\omega\\ &=\sum_{s\sigma}\sigma\frac{1}{\pi}\int d\omega\,\frac{\partial f}{\partial\omega}\delta_{s\sigma}(\omega)\ , \end{aligned} \tag{B13}$$

which yields the result (19) on putting $\partial f/\partial\omega = -\delta(\omega-\mu)$ as $T \rightarrow 0$.

The results used in Sec. V are obtained in an exactly analogous fashion. The perturbed Green's functions are no longer diagonal in spin space and it is convenient to introduce Green's functions $g_s^{ij}(z)$ which are 2×2 matrices in spin space. The corresponding unperturbed Green's functions take the form

$$\underline{G}_s^{ij} = \begin{pmatrix} G_{s\uparrow}^{ij} & 0 \\ 0 & G_{s\downarrow}^{ij} \end{pmatrix} . \tag{B14}$$

One finds analogous to (B3)

$$\underline{g}_s^{ij} = \underline{G}_s^{ij} + \underline{G}_s^{i0}(1-\underline{V}\,\underline{G}_s)^{-1}\underline{V}\,\underline{G}_s^{0j} , \tag{B15}$$

wher$\underline{V}$, $\underline{G}_s$ are defined at Eq. (26) and Eq. (27), and analogous to Eq. (B5)

$$\frac{\partial F}{\partial \mathrm{v}} = i\beta^{-1}\mathrm{v}^{-1}\sum_s\sum_\nu \mathrm{tr}\,\underline{V}\,\underline{g}_s^{00}(\omega_\nu) , \tag{B16}$$

where $\mathrm{v} = |\vec{\mathrm{v}}|$ and tr means the trace over spin space. Substituting Eq. (B15) into Eq. (B16) we have

$$\frac{\partial F}{\partial \mathrm{v}} = i\beta^{-1}\mathrm{v}^{-1}\sum_s\sum_\nu \mathrm{tr}\,\underline{V}\,\underline{G}_s(1-\underline{V}\,\underline{G}_s)^{-1} , \tag{B17}$$

which can be integrated to give

$$\Delta F = -i\beta^{-1}\sum_s\sum_\nu \mathrm{tr}\ln[1-\underline{V}\,\underline{G}_s(\omega_\nu)] . \tag{B18}$$

Converting the ν sum to a contour integral around the real axis and taking $T \rightarrow 0$ the results (24)−(27) follow.

---

[1] C. Herring, in *Magnetism*, edited by G.T. Rado and H. Suhl (Academic, New York, 1966) Vol. IV, Chap. VI.

[2] T. Moriya and A. Kawabata, J. Phys. Soc. Jpn. 34, 639 (1973).

[3] M.A. Klenin and J.A. Hertz, Phys. Rev. B 14, 3024 (1976).

[4] V. Korenman, J.L. Murray, and R.E. Prange, Phys. Rev. B 16, 4032 (1977).

[5] V. Korenman, J.L. Murray, and R.E. Prange, in Ref. 4, p. 4048.

[6] V. Korenman, J.L. Murray, and R.E. Prange, in Ref. 4, p. 4058.

[7] R.E. Prange and V. Korenman (unpublished).

[8] S.Q. Wang, W.E. Evanson, and J.R. Schrieffer, Phys. Rev. Lett. 23, 92 (1969).

[9] W.E. Evanson, J.R. Schrieffer, and S.Q. Wang, J. Appl. Phys. 41, 1199 (1970).

[10] J.R. Schrieffer, W.E. Evanson, and S.Q. Wang, J. Phys. (Paris) C 1, Supp. 2–3, Tome 32, 1 (1971).

[11] M. Cyrot, Phys. Rev. Lett. 25, 871 (1970).

[12] M. Cyrot, J. Phys. (Paris) 33, 125 (1972).

[13] P. Lacour-Gayet and M. Cyrot, J. Phys. C 7, 400 (1974).

[14] R.L. Stratonovitch, Dok. Akad. Nauk. SSSR 115, 1097 (1957), [Sov. Phys. Dokl. 2, 416 (1958)].

[15] J. Hubbard, Phys. Rev. Lett. 3, 77 (1959).

[16] R.A. Tawil and J. Callaway, Phys. Rev. B 7, 4242 (1972).

[17] S.H. Liu, Phys. Rev. B 15, 4281 (1977).

[18] D.R. Hamann, Phys. Rev. Lett. 23, 95 (1969).