

Pairing Treatment of Interacting Localized Moments in Dilute Magnetic Alloys*

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The Anderson model of a localized magnetic center is used to study a system of interacting localized moments in a dilute magnetic alloy. The effective interaction between centers, mediated by the conduction electrons, causes the localized quasiparticle energies to spread and lower by an amount proportional to $n_0^{1/2}$ (n_0 being the density of centers). The proportionality factor is greater by a factor of $2^{1/2}$ in the ferromagnetic state than in the paramagnetic state. Near these localized quasiparticle energies there are gaps in the conduction-band quasiparticle spectrum, the gaps being proportional to $n_0^{1/2}$. With the exception of the immediate vicinity of these gaps, the conduction-band quasiparticle spectrum is spread and shifted by an amount proportional to n_0 . These results are obtained by an equation-of-motion method that includes hole-electron pairing of a certain type. The latter allows one the flexibility of leaving unspecified the spin orientation of the electron occupying any given single-particle orbital.

I. INTRODUCTION

IN this paper we wish to study certain properties of an *interacting* system of localized moments in a dilute magnetic alloy. We represent each localized center containing a magnetic moment by the model of Anderson.¹ Each center contains localized one-electron levels of both signs of spin. The coupling between these levels and the conduction-band states causes the former to shift and to spread. For suitable values of the parameters of the model, it can also cause the spin degeneracy of the localized levels to lift. Under such conditions, a net localized magnetic moment forms.

A tremendous amount of theoretical effort has gone into attempts to understand the physical consequences of the Anderson model.^{2,3} Most of that effort has restricted itself to what is assumed to be the simplest case, a single localized center in an otherwise perfect crystal. A finite density of centers has been considered by Zuckermann⁴ in connection with the problem of effects of paramagnetic centers on superconductivity. A finite density was also considered by Caroli *et al.*⁵ in their treatment of electron spin resonance of dilute magnetic alloys. In neither case, however, was interaction between centers considered. Interaction between *two* centers was considered by Alexander and Anderson,⁶ and by Moriya.⁷

Here we wish to consider the interaction between

centers in the case where n_0 , the density of centers, is small but *finite*. Certain results we obtain are not at all obvious from the results of the two-center problem. Specifically, we find that there is a lowering and an additional spreading of the localized levels by an amount proportional to $n_0^{1/2}$. This occurs for both the paramagnetic and the ferromagnetic states, but the effect is $\sqrt{2}$ times as large in the latter case. As a consequence, the ferromagnetic state should be thermodynamically stable at sufficiently low temperatures. The conduction-band quasiparticle excitation spectrum is shifted by an amount proportional to n_0 , except in the immediate vicinity of one of the localized levels, where a gap in the spectrum appears, this gap being proportional to $n_0^{1/2}$. Lifetime effects are greatly enhanced immediately above each gap.

In the dilute-concentration limit, the effective interaction between centers is mediated by the conduction band and is of the Ruderman-Kittel type.⁸ We can visualize two centers interacting by virtue of exchanging an electron of arbitrary spin orientation through the intermediary of the conduction band. The probability amplitudes associated with electron emission from various centers may interfere with varying degrees of coherence and incoherence, depending on the state of each center at the time of emission. In this manner, the *net* interaction on any one center depends on the prior history of the states of all the other centers. The situation is somewhat analogous to Dicke's superradiant state,⁹ where gas atoms are coupled by the electromagnetic radiation field.

Because of the importance of *orientation* of electron spin in this problem, it is very convenient to introduce the idea of *pairing*. Specifically, one pairs an electron in some single-particle orbital, spin up, with a hole in the same single-particle orbital, spin down. Actually, all this amounts to is leaving unspecified the orientation of the spin of the electron occupying the single-particle orbital. The meaning of this becomes apparent in Sec.

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¹ P. W. Anderson, Phys. Rev. **124**, 41 (1961).

² For a review of efforts, as of the summer of 1967, see P. W. Anderson, in *Many-Body Physics*, edited by C. DeWitt and R. Balian (Gordon and Breach, Science Publishers, Inc., New York, 1968), p. 231.

³ For two of the most recent efforts, see S. Q. Wang, W. E. Evenson, and J. R. Schrieffer, Phys. Rev. Letters **23**, 92 (1969); D. R. Hamann, *ibid.* **23**, 95 (1969).

⁴ M. J. Zuckermann, Phys. Rev. **140**, A899 (1965).

⁵ B. Caroli, C. Caroli, and D. R. Fredkin, Phys. Rev. **178**, 599 (1969).

⁶ S. Alexander and P. W. Anderson, Phys. Rev. **133**, A1594 (1964).

⁷ T. Moriya, in *Proceedings of the International School of Physics "Enrico Fermi," Course XXXVII*, edited by W. Marshall (Academic Press Inc., New York, 1967), p. 206.

⁸ M. A. Ruderman and C. Kittel, Phys. Rev. **96**, 99 (1954).

⁹ R. H. Dicke, Phys. Rev. **93**, 99 (1954).

II, where we set up an operator equation-of-motion method¹⁰ for treating our problem. Similar (but not identical) hole-electron pairing also occurs in the problem of the hypothetical excitonic insulator.¹¹ However, the physical consequences of the pairing in the two cases are very different indeed.

II. EQUATIONS OF MOTION

The Hamiltonian of our system is

$$H = H_0 + H_1, \quad (2.1)$$

$$H_0 = \sum_{k,\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \epsilon_0 \sum_{i,\sigma} c_{i\sigma}^\dagger c_{i\sigma} + U_0 \sum_i c_{i\uparrow}^\dagger c_{i\uparrow} c_{i\downarrow}^\dagger c_{i\downarrow}, \quad (2.2)$$

$$H_1 = \sum_{k,i,\sigma} \{ V_{ki} c_{k\sigma}^\dagger c_{i\sigma} + V_{-ki} c_{i\sigma}^\dagger c_{k\sigma} \}. \quad (2.3)$$

The one-electron energies ϵ_k (for the conduction band) and ϵ_0 (for the localized centers) are measured relative to the Fermi level. The total Hamiltonian represents a system of conduction-band electrons interacting with electrons in localized s orbitals¹² on impurity centers, the index i designating centers. The positive Coulomb energy U_0 is associated with any center containing two opposite-spin localized electrons. We take

$$V_{ki}^* = V_{-ki}, \quad (2.4)$$

so that H_1 is Hermitian. We later need the fact that V_{ki} has the form

$$V_{ki} = V_k e^{-i\mathbf{k} \cdot \mathbf{R}_i}, \quad (2.5)$$

where \mathbf{R}_i is the position of the i th center and V_k is the matrix element for a center located at the origin. If we had only one center in the whole crystal, H would be the Hamiltonian for the Anderson model¹ of a localized magnetic center.

The electron creation and destruction operators obey the usual anticommutation relations

$$\begin{aligned} [c_{l\sigma}, c_{l'\sigma'}^\dagger]_+ &= \delta_{ll'} \delta_{\sigma\sigma'}, \\ [c_{l\sigma}, c_{l'\sigma'}]_+ &= [c_{l\sigma}^\dagger, c_{l'\sigma'}^\dagger]_+ = 0. \end{aligned} \quad (2.6)$$

Here we are using the notation

$$\{l\} = \{k\} + \{i\}, \quad (2.7)$$

¹⁰ The method of Sec. II is a modified version of an equation-of-motion technique, including pairing, developed by R. H. Parmenter, Phys. Rev. B 1, 1071 (1970).

¹¹ See, e.g., R. H. Parmenter and W. R. Henson, Phys. Rev. (to be published).

¹² We choose each center to be orbitally nondegenerate for reasons of simplicity. By a suitable replacement of the portion of H_0 associated with each center, we can generalize the theory to $(2l+1)$ -fold orbitally degenerate centers. In making this replacement, however, it is important to use the spherically symmetric center Hamiltonian of Caroli *et al.* (Ref. 5) rather than the one originally suggested by Anderson (Ref. 1) for describing a $(2l+1)$ -fold orbitally degenerate center. The lack of spherical symmetry of the latter Hamiltonian leads to certain difficulties in a hole-electron pairing theory.

i.e., the set of indices l represents the sum of the indices k plus the indices i .

We wish to look for an operator Θ such that

$$[\Theta, H] = \hbar\omega\Theta. \quad (2.8)$$

If Eq. (2.8) is exactly satisfied, $\hbar\omega$ is necessarily *real*. If $\hbar\omega$ is *positive*, Θ is a quasiparticle *destruction* operator associated with an excited state of the system containing one quasiparticle of energy $\hbar\omega$. If $\hbar\omega$ is *negative*, Θ is a quasiparticle *creation* operator associated with an excited state of the system containing one quasiparticle of energy $|\hbar\omega|$. If Eq. (2.8) is only approximately satisfied, then $\hbar\omega$ may be *complex*. In this case, the signature of the real part of $\hbar\omega$ determines whether Θ is a quasiparticle creation or destruction operator. In any case, $\hbar\omega$ must be in either the second or the fourth quadrant of the complex ω plane to ensure that the quasiparticle excitations are *causal* (i.e., decay with increasing time).

We assume that Θ can be written in the form

$$\Theta = \sum_{l,\sigma} a_{l\sigma}^* c_{l\sigma}, \quad (2.9)$$

where the $a_{l\sigma}^*$ are arbitrary coefficients. If we introduce the column vectors

$$A_l = \begin{pmatrix} a_{l\uparrow} \\ a_{l\downarrow} \end{pmatrix}, \quad \Psi_l = \begin{pmatrix} c_{l\uparrow} \\ c_{l\downarrow} \end{pmatrix}, \quad (2.10)$$

then Eq. (2.9) becomes

$$\Theta = \sum_l A_l^\dagger \Psi_l. \quad (2.11)$$

We have need of the general matrix notation

$$\begin{aligned} P &= \begin{pmatrix} p_\uparrow \\ p_\downarrow \end{pmatrix}, & P^\dagger &= (p_\uparrow^\dagger, p_\downarrow^\dagger), \\ M &= \begin{pmatrix} m_{\uparrow\uparrow} & m_{\uparrow\downarrow} \\ m_{\downarrow\uparrow} & m_{\downarrow\downarrow} \end{pmatrix}, & M^\dagger &= \begin{pmatrix} m_{\uparrow\uparrow}^\dagger & m_{\downarrow\uparrow}^\dagger \\ m_{\uparrow\downarrow}^\dagger & m_{\downarrow\downarrow}^\dagger \end{pmatrix}. \end{aligned} \quad (2.12)$$

An arbitrary M can be expanded in terms of the four matrices

$$\begin{aligned} \tau_1 &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, & i\tau_2 &= \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \\ \tau_3 &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, & \tau_4 &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \end{aligned} \quad (2.13)$$

If P and Q are two column vectors, we define

$$\begin{aligned} [P; Q]_+ &= \begin{pmatrix} [p_\uparrow, q_\uparrow]_+ & [p_\uparrow, q_\downarrow]_+ \\ [p_\downarrow, q_\uparrow]_+ & [p_\downarrow, q_\downarrow]_+ \end{pmatrix}, \\ [P; Q^\dagger]_+ &= \begin{pmatrix} [p_\uparrow, q_\uparrow^\dagger]_+ & [p_\uparrow, q_\downarrow^\dagger]_+ \\ [p_\downarrow, q_\uparrow^\dagger]_+ & [p_\downarrow, q_\downarrow^\dagger]_+ \end{pmatrix}. \end{aligned} \quad (2.14)$$

Thus Eq. (2.6) can be written

$$\begin{aligned} [\Psi_l; \Psi_{l'}^\dagger]_+ &= \delta_{ll'} \tau_4, \\ [\Psi_l; \Psi_{l'}]_+ &= 0. \end{aligned} \quad (2.15)$$

We also need the notation

$$K(l, l'; H) \equiv \langle [[\Psi_l, H]; \Psi_{l'}^\dagger]_+ \rangle, \quad (2.16)$$

where the angular brackets denote a thermal average. We assume that the only nonvanishing thermal averages are

$$\begin{aligned} n_{l\sigma} &\equiv \langle c_{l\sigma}^\dagger c_{l\sigma} \rangle, \\ b_l &\equiv \langle c_{l\uparrow}^\dagger c_{l\uparrow} \rangle. \end{aligned} \quad (2.17)$$

The assumption of finite b_l introduces the possibility of *pairing*. Here is it hole-electron pairing, as in the excitonic insulator,¹¹ rather than electron-electron pairing, as in the superconductor.¹³ In our problem, a finite b_l indicates only that an electron occupies orbital l with its spin pointing neither straight up nor straight down.

In order to solve Eq. (2.8), we need to evaluate $[\Psi_l, H]$. We make the approximation of *linearizing* $[\Psi_l, H]$; i.e., we take

$$[\Psi_l, H] = \sum_{l'} K(l, l'; H) \Psi_{l'}. \quad (2.18)$$

We are, in effect, following the prescription of Roth.¹⁴ Substituting (2.11) and (2.18) into (2.8), taking the anticommutator of the equation with $\Psi_{l'}^\dagger$, and making use of (2.15), we get

$$\sum_l A_l^\dagger \{ K(l, l'; H) - \hbar\omega \delta_{ll'} \tau_4 \} = 0. \quad (2.19)$$

We now make use of the specific form of the Hamiltonian in order to evaluate $K(l, l'; H)$. We define

$$u_i = \frac{1}{2} U_0 (n_{i\downarrow} - n_{i\uparrow}), \quad (2.20)$$

$$v_i = \epsilon_0 + \frac{1}{2} U_0 (n_{i\downarrow} + n_{i\uparrow}), \quad (2.21)$$

$$\Delta_i = U_0 b_i. \quad (2.22)$$

We obtain

$$K(k, k'; H_0) = \delta_{kk'} \epsilon_k \tau_4, \quad (2.23)$$

$$K(i, i'; H_0) = \delta_{ii'} \left\{ -\frac{1}{2} (\Delta_i + \Delta_i^*) \tau_1 - \frac{1}{2} (\Delta_i - \Delta_i^*) i \tau_2 + u_i \tau_3 + v_i \tau_4 \right\}, \quad (2.24)$$

$$K(k, i; H_0) = K(i, k; H_0) = 0, \quad (2.25)$$

$$K(k, k'; H_1) = K(i, i'; H_1) = 0, \quad (2.26)$$

$$K(k, i; H_1) = V_{ki} \tau_4, \quad (2.27)$$

$$K(i, k; H_1) = V_{ki}^* \tau_4. \quad (2.28)$$

Note that the thermal averages $n_{k\sigma}$ and b_k appear nowhere in the K 's, and thus nowhere in (2.19). The

equations of motion can now be written

$$\begin{aligned} A_i^\dagger \{ K(i, i; H_0) - \hbar\omega \tau_4 \} + \sum_{k'} A_{k'}^\dagger V_{k'i} &= 0, \\ A_k^\dagger (\epsilon_k - \hbar\omega) + \sum_{i'} A_{i'}^\dagger V_{ki}^* &= 0. \end{aligned} \quad (2.29)$$

We can immediately eliminate the A_k^\dagger 's in terms of the $A_{i'}^\dagger$'s, or vice versa. Thus

$$\begin{aligned} A_i^\dagger \{ K(i, i; H_0) - \hbar\omega \tau_4 - \sum_k |V_{ki}|^2 (\epsilon_k - \hbar\omega)^{-1} \tau_4 \} \\ - \sum_{i' \neq i} A_{i'}^\dagger \sum_k V_{ki}^* V_{k'i} (\epsilon_k - \hbar\omega)^{-1} \tau_4 &= 0, \end{aligned} \quad (2.30)$$

$$\begin{aligned} A_k^\dagger \{ (\epsilon_k - \hbar\omega) \tau_4 - \sum_i |V_{ki}|^2 [K(i, i; H_0) - \hbar\omega \tau_4]^{-1} \} \\ - \sum_{k' \neq k} A_{k'}^\dagger \sum_i V_{ki}^* V_{k'i} [K(i, i; H_0) - \hbar\omega \tau_4]^{-1} &= 0. \end{aligned} \quad (2.31)$$

In Eq. (2.30), the term

$$-\sum_k |V_{ki}|^2 (\epsilon_k - \hbar\omega)^{-1} \tau_4 = -\sum_k |V_k|^2 (\epsilon_k - \hbar\omega)^{-1} \tau_4 \quad (2.32)$$

represents a self-energy of a localized electron due to interaction with the conduction electrons. Here we have made use of Eq. (2.5) to show that this self-energy is the same for all centers. Being proportional to τ_4 , it is independent of the spin of the electron. In Eq. (2.30), the term

$$\begin{aligned} -\sum_k V_{ki}^* V_{k'i} (\epsilon_k - \hbar\omega)^{-1} \tau_4 = -\sum_k |V_k|^2 e^{ik \cdot (\mathbf{R}_i' - \mathbf{R}_i)} \\ \times (\epsilon_k - \hbar\omega)^{-1} \tau_4 \end{aligned} \quad (2.33)$$

represents the scattering of an electron from one localized site to another, via the intermediary of the conduction band. Being proportional to τ_4 , it is strictly potential scattering. In Eq. (2.31), the term

$$\begin{aligned} -\sum_i |V_{ki}|^2 [K(i, i; H_0) - \hbar\omega \tau_4]^{-1} \\ = -|V_k|^2 \sum_i [K(i, i; H_0) - \hbar\omega \tau_4]^{-1} \end{aligned} \quad (2.34)$$

represents the self-energy of a conduction electron due to interaction with the centers. Since it contains terms proportional to τ_1 , τ_2 , and τ_3 , this self-energy depends on the orientation of the spin of the conduction electron. In Eq. (2.31), the term

$$\begin{aligned} -\sum_i V_{ki}^* V_{k'i} [K(i, i; H_0) - \hbar\omega \tau_4]^{-1} = -V_k^* V_{k'} \\ \times \sum_i e^{i/(\mathbf{k} - \mathbf{k}') \cdot \mathbf{R}_i} [K(i, i; H_0) - \hbar\omega \tau_4]^{-1} \end{aligned} \quad (2.35)$$

represents the scattering of an electron from one Bloch state to another, via the intermediary of the localized sites. Since it contains terms proportional to τ_1 , τ_2 , and

¹³ J. Bardeen, L. N. Cooper, and J. R. Schrieffer, Phys. Rev. **108**, 1175 (1957).

¹⁴ L. M. Roth, Phys. Rev. Letters **20**, 1431 (1968).

τ_3 , the scattering depends on spin orientation and may involve spin flip.

III. LOCALIZED QUASIPARTICLES

We look for a solution to Eq. (2.30) where one particular vector coefficient, say A_i^\dagger , is much larger than all the others $A_{i'}^\dagger$. Equation (2.30) can be supplemented by the equation for $A_{i'}^\dagger$ ($i' \neq i$),

$$\begin{aligned} A_{i'}^\dagger \{K(i', i'; H_0) - \hbar\omega\tau_4 - \sum_k |V_k|^2 (\epsilon_k - \hbar\omega)^{-1} \tau_4\} \\ = \sum_{i'' \neq i'} A_{i''}^\dagger \sum_{k'} |V_{k'}|^2 e^{-ik' \cdot (R_{i'} - R_{i''})} (\epsilon_{k'} - \hbar\omega)^{-1} \tau_4 \\ \cong A_i^\dagger \sum_{k'} |V_{k'}|^2 e^{-ik' \cdot (R_i - R_{i'})} (\epsilon_{k'} - \hbar\omega)^{-1} \tau_4. \end{aligned} \quad (3.1)$$

In assuming $A_{i'}^\dagger$ much smaller than A_i^\dagger , we are making implicit use of the fact that n_0 , the density of localized centers, is small. Substituting (3.1) into (2.30), we get

$$A_i^\dagger \{G_i - P_i\} = 0, \quad (3.2)$$

where we define

$$G_i \equiv K(i, i; H_0) - (W + \hbar\omega)\tau_4, \quad (3.3)$$

$$\begin{aligned} W &\equiv \sum_k |V_k|^2 (\epsilon_k - \hbar\omega)^{-1} \\ &= (2\pi)^{-3} \int d^3k |V_k|^2 (\epsilon_k - \hbar\omega)^{-1}, \quad (3.4) \\ P_i &\equiv \sum_{k'} |V_{k'}|^2 (\epsilon_{k'} - \hbar\omega)^{-1} \sum_{i' \neq i} |V_{k'}|^2 (\epsilon_{k'} - \hbar\omega)^{-1} \\ &\quad \times \sum_{i' \neq i} G_{i'}^{-1} e^{i(k-k') \cdot (R_{i'} - R_i)} \\ &= (2\pi)^{-6} \int \int d^3k d^3k' |V_k|^2 |V_{k'}|^2 (\epsilon_k - \hbar\omega)^{-1} \\ &\quad \times (\epsilon_{k'} - \hbar\omega)^{-1} \sum_{i' \neq i} G_{i'}^{-1} e^{i(k-k') \cdot (R_{i'} - R_i)}. \end{aligned} \quad (3.5)$$

In these last two equations, we have replaced the k sums by the equivalent integrations. From (2.24) and (3.3), we get

$$G_i = -\frac{1}{2}(\Delta_i + \Delta_i^*)\tau_1 - \frac{1}{2}(\Delta_i - \Delta_i^*)i\tau_2 + u_i\tau_3 + (v_i - W - \hbar\omega)\tau_4, \quad (3.6)$$

so that

$$G_i^{-1} = \{(v_i - W - \hbar\omega)^2 - w_i^2\}^{-1} \{(v_i - W - \hbar\omega)\tau_4 - u_i\tau_3 + \frac{1}{2}(\Delta_i + \Delta_i^*)\tau_1 + \frac{1}{2}(\Delta_i - \Delta_i^*)i\tau_2\}. \quad (3.7)$$

Here we are introducing the notation

$$w_i \equiv (u_i^2 + |\Delta_i|^2)^{1/2}. \quad (3.8)$$

At this point, and only at this point, we need to anticipate certain results of the calculation. It turns out that v_i and w_i are always independent of the index i . In one of the two kinds of solution, u_i and Δ_i are also independent of i ; in the other kind of solution, u_i and

Δ_i vary in an essentially random fashion from site to site, subject to the constraint that w be site-independent. The former is the ordered solution; the latter is the disordered solution. We define

$$\begin{aligned} I_i &\equiv (2\pi)^{-6} \int \int d^3k d^3k' |V_k|^2 |V_{k'}|^2 (\epsilon_k - \hbar\omega)^{-1} \\ &\quad \times (\epsilon_{k'} - \hbar\omega)^{-1} \sum_{i' \neq i} e^{i(k-k') \cdot (R_{i'} - R_i)}, \end{aligned} \quad (3.9)$$

$$D_i \equiv \{(v_i - W - \hbar\omega)^2 - w_i^2\}^{-1} (v_i - W - \hbar\omega)\tau_4. \quad (3.10)$$

I_i differs from P_i by the absence of $G_{i'}^{-1}$. D_i is that portion of G_i^{-1} proportional to τ_4 . For the ordered solution, we can replace $G_{i'}^{-1}$ by G_i^{-1} in P_i , so that

$$P_i = G_i^{-1} I_i. \quad (3.11)$$

For the disordered solution, the portions of $G_{i'}^{-1}$ proportional to τ_1 , τ_2 , and τ_3 make negligible contributions to the sum over i' in P_i , this being because of the random nature of u_i and Δ_i . The portion of $G_{i'}^{-1}$ proportional to τ_4 is equal to D_i so that

$$P_i = D_i I_i. \quad (3.12)$$

We can now rewrite (3.2) as

$$A_i^\dagger G_i' = 0, \quad (3.13)$$

where we are defining

$$\begin{aligned} G_i' &\equiv -\frac{1}{2}(\Delta_i + \Delta_i^*)\tau_1 - \frac{1}{2}(\Delta_i - \Delta_i^*)i\tau_2 + u_i\tau_3 \\ &\quad + \alpha_i(v_i - W - \hbar\omega)\tau_4, \end{aligned} \quad (3.14)$$

$$\alpha_i \equiv \frac{(v_i - W - \hbar\omega)^2 - w_i^2 - I_i}{(v_i - W - \hbar\omega)^2 - w_i^2 + qI_i}, \quad (3.15)$$

and the parameter q is defined as

$$\begin{aligned} q &= +1 \quad \text{ordered state} \\ &= 0 \quad \text{disordered state.} \end{aligned} \quad (3.16)$$

In other words, G_i' differs from G_i only in that τ_4 is replaced by $\alpha_i\tau_4$. The degree of order of the state manifests itself only in the renormalization factor α_i .

In order to evaluate W , we make the usual replacement

$$\hbar\omega \rightarrow \hbar\omega + i\eta_\omega, \quad (3.17)$$

where η_ω is an infinitesimal having the same signature as the real part of ω . This implies that

$$\omega = \omega_1 - i\omega_2 \quad (3.18)$$

will lie in either the second or the fourth quadrant of the complex ω plane, as has already been discussed. Making use of the formal relation

$$\lim_{\eta \rightarrow 0^+} (x \pm i\eta)^{-1} = \mathcal{P}(1/x) \mp i\pi\delta(x), \quad (3.19)$$

where \mathcal{P} denotes "principal part of," we can evaluate (3.4). Writing

$$W = W_1 - iW_2, \quad (3.20)$$

we have

$$W_1 = (2\pi)^{-1} \mathcal{P} \int d^3k |V_k|^2 (\epsilon_k - \hbar\omega_1)^{-1}, \quad (3.21)$$

$$W_2 = -\frac{1}{2}(2\pi)^{-2} (\text{sgn}\omega_1) \int d^3k |V_k|^2 \delta(\epsilon_k - \hbar\omega_1). \quad (3.22)$$

It is often a good approximation to neglect the ω dependence of W by setting $\omega_1 = 0$ in the integrands of Eqs. (3.21) and (3.22).

In order to evaluate I_i , we approximate the sum over $i' \neq i$ by the equivalent integral,

$$\sum_{i' \neq i} e^{i(\mathbf{k}-\mathbf{k}') \cdot (\mathbf{R}_i - \mathbf{R}_{i'})} = n_0 \int d^3R e^{i(\mathbf{k}-\mathbf{k}') \cdot \mathbf{R}}. \quad (3.23)$$

(We are assuming a crystal of unit volume.) Note that, having made this approximation, $I_i = I$ is independent of the index i . To aid in evaluating Eq. (3.9), we introduce the convergence factor

$$\lim_{K \rightarrow 0} 3(KR)^{-1} j_1(KR) = 1, \quad (3.24)$$

where j_1 is the spherical Bessel function of order 1. The point of doing this is that

$$\begin{aligned} n_0 \int d^3R 3(KR)^{-1} j_1(KR) e^{i(\mathbf{k}-\mathbf{k}') \cdot \mathbf{R}} \\ = n_0 \left(\frac{4}{3} \pi K^3 \right)^{-1} \quad \text{if } |\mathbf{k}-\mathbf{k}'| < K \\ = 0 \quad \text{otherwise.} \end{aligned} \quad (3.25)$$

Making use of

$$\begin{aligned} (\epsilon_k - \hbar\omega)^{-1} (\epsilon_{k'} - \hbar\omega)^{-1} &= (\epsilon_{k'} - \epsilon_k)^{-1} \\ &\times [(\epsilon_k - \hbar\omega)^{-1} - (\epsilon_{k'} - \hbar\omega)], \end{aligned} \quad (3.26)$$

we can write (3.9) as

$$\begin{aligned} I &= \lim_{K \rightarrow 0} (2\pi)^{-6} n_0 \left(\frac{4}{3} \pi K^3 \right)^{-1} \int \int_{|\mathbf{k}-\mathbf{k}'| < K} d^3k d^3k' |V_k|^2 \\ &\times |V_{k'}|^2 2(\epsilon_{k'} - \epsilon_k)^{-1} (\epsilon_k - \hbar\omega)^{-1}. \end{aligned} \quad (3.27)$$

We have

$$(\epsilon_{k'} - \epsilon_k) = 2\kappa(\hbar^2 k^2 / 2m) [(\kappa/2k) - \mu], \quad (3.28)$$

where $\kappa = \mathbf{k} - \mathbf{k}'$, μ is the cosine of the angle between κ and \mathbf{k} , and m is the conduction-band effective mass. Thus

$$\begin{aligned} I &= \lim_{K \rightarrow 0} (2\pi)^{-6} n_0 \left(\frac{4}{3} \pi K^3 \right)^{-1} \int d^3k |V_k|^4 (\epsilon_k - \hbar\omega)^{-1} \\ &\times (\hbar^2 k^2 / 2m)^{-1} \int_0^K 2\pi\kappa d\kappa \int_{-1}^1 [(\kappa/2k) - \mu]^{-1} d\mu. \end{aligned} \quad (3.29)$$

Taking the principal part of the μ integration, in the limit of small K we get

$$\begin{aligned} &\int_0^K 2\pi\kappa d\kappa \mathcal{P} \int_{-1}^1 [(\kappa/2k) - \mu]^{-1} d\mu \\ &= \int_0^K 2\pi\kappa d\kappa \ln \left[\frac{1 + (\kappa/2k)}{1 - (\kappa/2k)} \right] \\ &= 4\pi \int_0^K (\kappa/2k) \kappa d\kappa = (2k)^{-1} \left(\frac{4}{3} \pi K^3 \right), \end{aligned} \quad (3.30)$$

so that

$$I = \frac{1}{2} n_0 (2\pi)^{-6} \int d^3k |V_k|^4 (\hbar^2 k^2 / 2m)^{-1} (\epsilon_k - \hbar\omega)^{-1}. \quad (3.31)$$

Note that $(\hbar^2 k^2 / 2m)^{-1}$ causes no singularity in the integrand at $\mathbf{k} = 0$. Evaluating this by the same procedure used for W , we get

$$I = I_1 - iI_2, \quad (3.32)$$

where

$$I_1 = \frac{1}{2} n_0 (2\pi)^{-6} \mathcal{P} \int d^3k |V_k|^4 (\hbar^2 k^2 / 2m)^{-1} \times (\epsilon_k - \hbar\omega_1)^{-1}, \quad (3.33)$$

$$I_2 = -\frac{1}{4} n_0 (2\pi)^{-5} (\text{sgn}\omega_1) \int d^3k |V_k|^4 (\hbar^2 k^2 / 2m)^{-1} \times \delta(\epsilon_k - \hbar\omega_1). \quad (3.34)$$

As with W , it is often a good approximation to ignore the ω dependence of I . Note that both W and I lie in either the first or the fourth quadrant of the complex plane.

We return to Eq. (3.13). Corresponding to this pair of linear equations, there is the secular equation

$$\begin{vmatrix} \alpha_i(v_i - W - \hbar\omega) + u_i & -\Delta_i \\ -\Delta_i^* & \alpha_i(v_i - W - \hbar\omega) - u_i \end{vmatrix} = 0, \quad (3.35)$$

which gives

$$\alpha_i(v_i - W - \hbar\omega) \pm w_i = 0. \quad (3.36)$$

Substituting (3.36) back into (3.15), we get an equation cubic in α_i^{-1} ,

$$\alpha_i^{-3} - \alpha_i^{-2} - [1 + (I/w_i^2)] \alpha_i^{-1} + [1 - q(I/w_i^2)] = 0. \quad (3.37)$$

Solving for the roots in the usual fashion, expanding in powers of (I/w_i^2) , and keeping only the leading terms, we get

$$\alpha_i^{-1} = -1 \quad (3.38)$$

and

$$\alpha_i^{-1} = 1 \mp w_i^{-1} [\frac{1}{2}(1+q)I]^{1/2}. \quad (3.39)$$

The root given by (3.38) is unacceptable in that it does not reduce to $+1$ in the limit as n_0 and I go to zero. The two roots given by (3.39) are acceptable in this regard. We must, however, have the sign appearing in (3.39) be opposite to that appearing in (3.36). This en-

sures that ω lies in either the second or fourth quadrant, as can be seen by substituting (3.39) into (3.36) and getting¹⁵

$$\hbar\omega = v_i - W \pm \alpha_i^{-1} w_i = v_i - W \pm w_i - [\frac{1}{2}(1+q)I]^{1/2}. \quad (3.40)$$

(Here we take the square root of I that lies in the same quadrant as I .)

If we think of V_k as being proportional to a coupling constant g , then $-W$ and $-I^{1/2}$ are both proportional to g^2 . However, $-W$ is independent of n_0 , whereas $-I^{1/2}$ is proportional to $n_0^{1/2}$. Finally, we note that $-\frac{1}{2}(1+q)I^{1/2}$ is larger by a factor of $\sqrt{2}$ in the ordered phase than it is in the disordered phase.

We introduce the notation

$$A_{i\pm}^\dagger = (a_{i\pm}^*, a_{i\pm}^\dagger), \quad (3.41)$$

the \pm sign being the same as that of Eqs. (3.36) and (3.40). Equation (3.13) becomes

$$(a_{i\pm}^*, a_{i\pm}^\dagger) \begin{pmatrix} \pm w_i - u_i & \Delta_i \\ \Delta_i^* & \pm w_i + u_i \end{pmatrix} = 0. \quad (3.42)$$

Solving this, we get

$$\begin{aligned} a_{i\pm}^* &= a_{i\pm}^\dagger = C_i^{-1}(w_i + u_i), \\ a_{i\pm}^\dagger &= -a_{i\pm}^* = -C_i^{-1}\Delta_i, \\ C_i &\equiv [2w_i(w_i + u_i)]^{1/2}. \end{aligned} \quad (3.43)$$

Following the procedure of Ref. 10, we define the square matrix U^{-1} such that

$$U^{-1} \equiv \begin{pmatrix} A_{i+}^\dagger \\ A_{i-}^\dagger \end{pmatrix} = \begin{pmatrix} a_{i+}^* & a_{i+}^\dagger \\ a_{i-}^* & a_{i-}^\dagger \end{pmatrix}. \quad (3.44)$$

Thus here we have

$$U = C_i^{-1} \begin{pmatrix} w_i + u_i & +\Delta_i \\ -\Delta_i^* & w_i + u_i \end{pmatrix}. \quad (3.45)$$

Making a trivial change in a proof of Ref. 10, we get

$$\begin{aligned} n_{i\uparrow} &= |U_{i\uparrow}|^2 f_+ + |U_{i\downarrow}|^2 f_-, \\ 1 - n_{i\downarrow} &= |U_{i\uparrow}|^2 (1 - f_+) + |U_{i\downarrow}|^2 (1 - f_-), \\ b_i &= U_{i\uparrow}^* U_{i\uparrow} f_+ + U_{i\downarrow}^* U_{i\downarrow} f_-, \end{aligned} \quad (3.46)$$

where

$$f_{\pm} \equiv \pi^{-1} |\omega_{2\pm}| \int d\omega' [(\omega' - \omega_{1\pm})^2 + \omega_{2\pm}^2]^{-1} \times [e^{\beta\hbar\omega'} + 1]^{-1}, \quad (3.47)$$

$\omega_{1\pm}$ and $-\omega_{2\pm}$ being the real and imaginary parts, respectively, of the roots ω_{\pm} of Eq. (3.40). Substituting

(3.45) into (3.46) gives

$$(n_{i\downarrow} + n_{i\uparrow}) = (f_- + f_+), \quad (3.48)$$

$$(n_{i\downarrow} - n_{i\uparrow}) = (u_i/w_i)(f_- - f_+), \quad (3.49)$$

$$b_i = \frac{1}{2}(\Delta_i/w_i)(f_- - f_+). \quad (3.50)$$

Substitution of these results into Eqs. (2.20)–(2.22) gives, respectively,

$$u_i = \frac{1}{2}U_0(u_i/w_i)(f_- - f_+), \quad (3.51)$$

$$v_i = \epsilon_0 + \frac{1}{2}U_0(f_- + f_+), \quad (3.52)$$

$$\Delta_i = \frac{1}{2}U_0(\Delta_i/w_i)(f_- - f_+). \quad (3.53)$$

Note that Eqs. (3.51) and (3.53) are the same equation. This means that u_i and Δ_i are not separately determinable. Subject only to Eq. (3.8) being satisfied, they are otherwise arbitrary. Of course u_i , by definition, is real, but Δ_i may be complex. In addition, these equations imply that $w_i = w$ and $v_i = v$ are both independent of i , as was promised. They may be determined by solving the coupled set of equations

$$v = \epsilon_0 + \frac{1}{2}U_0(f_- + f_+), \quad (3.54)$$

$$w = \frac{1}{2}U_0(f_- - f_+), \quad (3.55)$$

$$\hbar\omega_{\pm} = v \pm w - W - [\frac{1}{2}(1+q)I]^{1/2}, \quad (3.56)$$

f_{\pm} being determined from ω_{\pm} via Eq. (3.47). It is to be understood that the only acceptable solutions leading to $w=0$ are those for which $q=1$, as discussed in Ref. 15.

It is clear that

$$S_{zi} \equiv -\frac{1}{2}\hbar(n_{i\downarrow} - n_{i\uparrow}) = -(\hbar/U_0)u_i \quad (3.57)$$

is the z component of spin angular momentum on the i th site. This suggests that we make the association

$$S_{xi} - iS_{yi} = (\hbar/U_0)\Delta_i. \quad (3.58)$$

Thus the *magnitude* of the spin on any site is

$$S = (\hbar/U_0)w = \frac{1}{2}\hbar(f_- - f_+). \quad (3.59)$$

Note that this magnitude may be temperature-dependent. The nonuniqueness of u_i and Δ_i indicates that the spin of a site can be *arbitrarily oriented*, with this orientation being the same for all sites in the ordered phase ($q=1$), and the orientation being randomly different for different sites in the disordered phase ($q=0$). Thus the ordered phase is *ferromagnetic*, the disordered phase is *paramagnetic*. In the limit as $n_0 \rightarrow 0$, our coupled set of equations reduces exactly to those of Andreson¹ for a single isolated impurity.

IV. CONDUCTION-BAND QUASIPARTICLES

In Sec. III we examined the solution of Eq. (2.30); here we wish to do the same for Eq. (2.31). We look for a solution where one particular coefficient, say A_k^\dagger , is

¹⁵ It should be emphasized that Eq. (3.40), having been obtained by expanding in powers of (I/w_i^2) , is not correct when $w_i=0$. Under such conditions, $\hbar\omega$ must be independent of q , so that the appropriate solution of Eq. (3.36) is $\alpha_i=0$, or $\hbar\omega = v_i - W - I^{1/2}$. Thus we see that Eq. (3.40) gives the correct answer when $w_i=0$ if we set $q=1$ in the equation.

much larger than all the others $A_{k'}^\dagger$. Equation (2.31) can be supplemented by the equation for $A_{k'}^\dagger$ ($k' \neq k$),

$$\begin{aligned} A_{k'}^\dagger \{ (\epsilon_{k'} - \hbar\omega)\tau_4 - |V_{k'}|^2 \sum_i [K(i, i; H_0) - \hbar\omega\tau_4]^{-1} \} \\ = \sum_{k'' \neq k'} A_{k''}^\dagger V_{k''}^* V_{k'} \sum_i e^{i(\mathbf{k}' - \mathbf{k}'') \cdot \mathbf{R}_i} \\ \times [K(i, i; H_0) - \hbar\omega\tau_4]^{-1} \\ \cong A_k^\dagger V_{k'}^* V_k \sum_i e^{i(\mathbf{k}' - \mathbf{k}) \cdot \mathbf{R}_i} [K(i, i; H_0) - \hbar\omega\tau_4]^{-1}. \quad (4.1) \end{aligned}$$

Substituting (4.1) into (2.31), we get

$$A_k^\dagger \{ G_k - I_k \} = 0, \quad (4.2)$$

where we define

$$G_k \equiv (\epsilon_k - \hbar\omega)\tau_4 - |V_k|^2 \sum_i Q_i^{-1}, \quad (4.3)$$

$$Q_i \equiv K(i, i; H_0) - \hbar\omega\tau_4 = G_i + W\tau_4, \quad (4.4)$$

$$\begin{aligned} I_k \equiv |V_k|^2 \sum_{k' \neq k} |V_{k'}|^2 \sum_{i, i'} e^{i(\mathbf{k}' - \mathbf{k}) \cdot (\mathbf{R}_i - \mathbf{R}_{i'})} Q_i^{-1} G_{k'}^{-1} Q_{i'}^{-1} \\ = (2\pi)^{-3} |V_k|^2 \int d^3k' |V_{k'}|^2 \sum_i Q_i^{-1} G_{k'}^{-1} Q_i^{-1}. \quad (4.5) \end{aligned}$$

In the last line of (4.5), the double sum over i and i' reduces to a single sum over i , because of destructive interference when $i' \neq i$. To the accuracy of terms linear in n_0 , we can replace $G_{k'}^{-1}$ in (4.5) by $(\epsilon_{k'} - \hbar\omega)^{-1}\tau_4$, thereby getting

$$I_k = W |V_k|^2 \sum_i Q_i^{-2}, \quad (4.6)$$

where W is defined by Eq. (3.4). Since

$$\begin{aligned} Q_i^{-1} = [(v - \hbar\omega)^2 - w^2]^{-1} \left[1 + \frac{1}{2}(\Delta_i + \Delta_i^*)\tau_1 \right. \\ \left. + \frac{1}{2}(\Delta_i - \Delta_i^*)i\tau_2 - u_i\tau_3 + (v - \hbar\omega)\tau_4 \right], \quad (4.7) \end{aligned}$$

$$\begin{aligned} Q_i^{-2} = \frac{2(v - \hbar\omega)}{[(v - \hbar\omega)^2 - w^2]} \left[\frac{1}{2}(\Delta_i + \Delta_i^*)\tau_1 + \frac{1}{2}(\Delta_i - \Delta_i^*)i\tau_2 \right. \\ \left. - u_i\tau_3 \right] + \frac{(v - \hbar\omega)^2 + w^2}{[(v - \hbar\omega)^2 - w^2]^2} \tau_4, \quad (4.8) \end{aligned}$$

we have

$$\begin{aligned} \sum_i Q_i^{-1} = \frac{n_0(v - \hbar\omega)}{[(v - \hbar\omega)^2 - w^2]} \tau_4 + \frac{n_0 q}{[(v - \hbar\omega)^2 - w^2]} \\ \times \left[\frac{1}{2}(\Delta + \Delta^*)\tau_1 + \frac{1}{2}(\Delta - \Delta^*)i\tau_2 - u\tau_3 \right], \quad (4.9) \end{aligned}$$

$$\begin{aligned} \sum_i Q_i^{-2} = \frac{n_0[(v - \hbar\omega)^2 + w^2]}{[(v - \hbar\omega)^2 - w^2]^2} \tau_4 + \frac{2n_0(v - \hbar\omega)q}{[(v - \hbar\omega)^2 - w^2]^2} \\ \times \left[\frac{1}{2}(\Delta + \Delta^*)\tau_1 + \frac{1}{2}(\Delta - \Delta^*)i\tau_2 - u\tau_3 \right]. \quad (4.10) \end{aligned}$$

Thus

$$\begin{aligned} G_k - I_k = \left\{ (\epsilon_k - \hbar\omega) - \frac{n_0 |V_k|^2}{[(v - \hbar\omega)^2 - w^2]} \right. \\ \times \left[(v - \hbar\omega) + \left(\frac{(v - \hbar\omega)^2 + w^2}{(v - \hbar\omega)^2 - w^2} \right) W \right] \tau_4 \\ \left. - \frac{n_0 |V_k|^2 q}{[(v - \hbar\omega)^2 - w^2]} \left[1 + \left(\frac{2(v - \hbar\omega)W}{(v - \hbar\omega)^2 - w^2} \right) \right] \right. \\ \left. \times \left[\frac{1}{2}(\Delta + \Delta^*)\tau_1 + \frac{1}{2}(\Delta - \Delta^*)i\tau_2 - u\tau_3 \right] \right\}. \quad (4.11) \end{aligned}$$

Corresponding to Eq. (4.2), we have the secular equation

$$\det(G_k - I_k) = 0, \quad (4.12)$$

which gives

$$\begin{aligned} \hbar\omega = \epsilon_k - \frac{n_0 |V_k|^2}{[(v - \hbar\omega)^2 - w^2]} \left[(v - \hbar\omega) + \left(\frac{(v - \hbar\omega)^2 + w^2}{(v - \hbar\omega)^2 - w^2} \right) W \right] \\ \pm q \frac{n_0 |V_k|^2 w}{[(v - \hbar\omega)^2 - w^2]} \left[1 + \left(\frac{2(v - \hbar\omega)W}{(v - \hbar\omega)^2 - w^2} \right) \right]. \quad (4.13) \end{aligned}$$

Thus, for the disordered ($q=0$) phase, we have the doubly degenerate root

$$\begin{aligned} \hbar\omega = \epsilon_k - \frac{n_0 |V_k|^2}{[(v - \hbar\omega)^2 - w^2]} \\ \times \left[(v - \hbar\omega) + \left(\frac{(v - \hbar\omega)^2 + w^2}{(v - \hbar\omega)^2 - w^2} \right) W \right]. \quad (4.14) \end{aligned}$$

For the ordered ($q=1$) phase, we have

$$\hbar\omega = \epsilon_k - \frac{n_0 |V_k|^2}{[v - \hbar\omega \pm w]} \left[1 + \frac{W}{[v - \hbar\omega \pm w]} \right]. \quad (4.15)$$

In the disordered case, $\hbar\omega$ has gaps at $\epsilon_k = (v - w)$ and $\epsilon_k = (v + w)$. In the ordered case, $\hbar\omega_+$ has a gap at $\epsilon_k = (v + w)$, $\hbar\omega_-$ has a gap at $\epsilon_k = (v - w)$. Far, in energy, from these gaps, the shift in energy due to the finite density of centers is proportional to n_0 . Close to the gaps, the shift is proportional to $n_0^{1/3}$. We calculate the size of the gaps. Consider the ordered case. Setting $\epsilon_k = (v \pm w)$ in (4.15), we get

$$\hbar\omega = v \pm w - [n_0 |V_k|^2 W]^{1/3} \quad (4.16)$$

in the limit of small n_0 . Two of the three cube roots of W will satisfy the condition that ω lie in either the second or the fourth quadrant of the complex plane. These two choices for $W^{1/3}$ set the two values of $\hbar\omega$ which define the gap. Consider the case where $|W_2| \ll |W_1|$. Then we get

$$\begin{aligned} \hbar\omega = v \pm w - [n_0 |V_k|^2 |W_1|]^{1/3} \\ \times \left[1 + \frac{1}{3}i(\text{sgn}\omega_1) \frac{|W_2|}{|W_1|} \right] \quad (4.17) \end{aligned}$$

for the bottom of the gap, and

$$\hbar\omega = v \pm w + \frac{1}{2}[n_0 |V_k|^2 |W_1|]^{1/3} [1 - \sqrt{3}i(\text{sgn}\omega_1)] \quad (4.18)$$

for the top. Notice that the damping is much greater above the gap than below the gap. The real part of the gap has the value

$$\frac{3}{2}[n_0 |V_k|^2 |W_1|]^{1/3}.$$

Next consider the disordered case. Setting $\epsilon_k = (v \pm w)$ in (4.14), we get, in the limit of small n_0 ,

$$\hbar\omega = v \pm w - [\frac{1}{2}n_0 |V_k|^2 |W|]^{1/3}, \quad (4.19)$$

differing from (4.16) only by a factor of $2^{-1/3}$. Thus here the real part of the gap has the value

$$\frac{3}{2}[\frac{1}{2}n_0 |V_k|^2 |W|]^{1/3}.$$

We introduce the notation

$$A_{k\pm}^\dagger = (a_{k\pm}^{\uparrow*}, a_{k\pm}^{\downarrow*}), \quad (4.20)$$

the \pm sign being the same as that of Eqs. (4.13) and (4.15). Equation (4.2) becomes

$$(a_{k\pm}^{\uparrow*}, a_{k\pm}^{\downarrow*}) \begin{pmatrix} \pm w - u & \Delta \\ \Delta^* & \pm w + u \end{pmatrix} = 0. \quad (4.21)$$

Note that (4.21) has a form identical to that of (3.42). This means that we can go through the same kind of analysis developed in Sec. III, and will eventually get

$$(n_{k\downarrow} + n_{k\uparrow}) = (f_{k-} + f_{k+}), \quad (4.22)$$

$$(n_{k\downarrow} - n_{k\uparrow}) = (u/w)(f_{k-} - f_{k+}), \quad (4.23)$$

where $f_{k\pm}$ is obtained by substituting Eq. (4.13) into Eq. (3.47). For the disordered case, $f_{k\pm}$ is independent of \pm , so that $n_{k\sigma}$ is independent of σ , as it should be. For the ordered case, it is convenient to assume the localized magnetic moments are all parallel to the z

axis, so that $\Delta = 0$ and $u = w$. Now Eq. (4.23) becomes

$$(n_{k\downarrow} - n_{k\uparrow}) = (f_{k-} - f_{k+}), \quad (4.24)$$

while Eq. (3.49) becomes

$$(n_{i\downarrow} - n_{i\uparrow}) = (f_- - f_+). \quad (4.25)$$

Note that the signature of $(n_{i\downarrow} - n_{i\uparrow})$ is the same as that of $(\omega_{1+} - \omega_{1-})$, this being true of both the localized centers and of the conduction band. From Eq. (3.56), we see that this signature is always positive for the centers. From Eq. (4.15), on the other hand, we see that $(\omega_{1+} - \omega_{1-})$ for the conduction band will be *negative* when ω_{\pm} both lie *between* the two gaps already discussed. When ω_{\pm} lie above or below both gaps, the signature is *positive*. As was pointed out by Anderson,¹ the optimum conditions for maximizing the size of the moment of a center are that $(v - w)$ be below the Fermi level, $(v + w)$ be above. Under such conditions, $(n_{k\downarrow} - n_{k\uparrow})$ will be negative for k at or near the Fermi surface. But these are the only k for which the difference $(f_{k-} - f_{k+})$ can be appreciable in magnitude. Thus the net conduction-band magnetic moment will oppose that of the centers; i.e., the conduction electrons respond *antiferromagnetically* to the localized moments of the centers.¹⁶

With regard to concentration dependence, the quasiparticle energies of the conduction band vary more slowly with n_0 than do the quasiparticle energies of the centers, the former varying as n_0 , the latter as $n_0^{1/2}$. (We are ignoring the immediate vicinity of the gaps in the conduction band.) Therefore, in the low-density limit, the internal energy of the complete system should be lower for the ordered (ferromagnetic) state than for the disordered (paramagnetic) state, since the quasiparticle energies of the centers favor the former over the latter. We do not attempt, in this paper, a calculation of the n_0 dependence of the associated Curie temperature.

¹⁶ J. R. Schrieffer and P. A. Wolff, Phys. Rev. **149**, 491 (1966).