

The relation between the amplitudes of the electric field and of the acoustic displacement is found using the result

$$E_{\pm} = \frac{mi\omega}{e\tau} \frac{1 - \sigma_0 R_{\pm}}{1 - i\beta\sigma_0 R_{\pm}} \xi_{\pm}. \quad (55)$$

For the left-hand polarization we obtain (after making the same approximations that were made in Sec. II)

$$\xi_{+} = -[e(\omega g - \omega_H)/m\omega^2\omega_c]E_{+}. \quad (56)$$

In particular, for the crossing branches at the frequency ω_d we find the relation

$$\xi_{+} = \pm \frac{eg_d}{m\omega_d\omega_c} \left(\frac{\Omega_c}{2g_d\omega_d} \right)^{1/2} E_{+}, \quad (57)$$

where the \pm sign correspond to the two branches in Eq. (54). A simple calculation shows that at the cross-

over the elastic energy density is equal to the electromagnetic energy density as expected.

The strong coupling between helicon and transverse acoustic waves in the region of the crossover suggests the possibility of exciting the latter modes by electromagnetic means. It is, of course, also possible to use this effect for the detection of transverse acoustic modes. Finally, it is interesting to notice that for some values of the magnetic field Eq. (51) can have up to three solutions for w_d while ordinarily it only has one.

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Interaction Between Localized States in Metals

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The theory of localized magnetic states of solute atoms in metals is extended to the case of a pair of neighboring magnetic atoms. It is found that the simplified model based on the idea that the important interaction is the diagonal exchange integral in the localized state, which is exactly soluble in Hartree-Fock theory for isolated ions, is still soluble, and the solutions show both ferromagnetic and antiferromagnetic exchange mechanisms.

I. INTRODUCTION

THE nature of the localized magnetic impurity states observed in metals¹ was investigated in a number of recent papers.²⁻⁴ Following the ideas of Mott⁵ and Friedel⁶ on the nature of the magnetic state, it was shown that such states can be described as virtual localized states in the conduction band. Their magnetic behavior is dominated by the Coulomb repulsion between electrons of opposite spin in the same atomic

state.² The magnetism is therefore basically of atomic origin and in this sense resembles the truly localized magnetic moments in insulators.⁷ The situation in metals differs from that in insulators because the localized states are virtual, i.e., spread out in energy because of $s-d$ interactions, and can therefore contain a nonintegral number of electrons. As a result they describe something intermediate between a localized and an itinerant situation. The magnetic properties are essentially those of localized states whereas the effects on the electronic specific heat are similar to those of an itinerant density of states at the Fermi level.

The purpose of the present paper is to try to calculate the interaction between two similar magnetic impurities near to each other in an otherwise completely nonmagnetic material. Like the cases of a single impurity

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¹ B. T. Matthias, M. Peter, H. J. Williams, A. M. Clogston, E. Corenzwit, and R. J. Sherwood, *Phys. Rev. Letters* **5**, 542 (1960); *Phys. Rev.* **125**, 541 (1962).

² P. W. Anderson, *Phys. Rev.* **124**, 41 (1961).

³ P. A. Wolff, *Phys. Rev.* **124**, 1030 (1961).

⁴ A. M. Clogston, *Phys. Rev.* **125**, 439 (1962).

⁵ N. F. Mott, *Proc. Phys. Soc. (London)* **A62**, 416 (1949).

⁶ J. Friedel, *Suppl. Nuovo Cimento* **7**, 287 (1958); A. Blandin and J. Friedel, *J. Phys. Radium* **20**, 160 (1958).

⁷ For a discussion of these ideas see, e.g., Ref. 13.

and of the pure magnetic metal, this case can, in principle, be solved exactly within the Hartree-Fock method. The results, in contrast to both of the other two cases, can then be reasonably directly interpreted in terms of exchange processes taking place between the magnetic atoms, and in particular ferro- and antiferromagnetic and indirect exchange processes can be easily identified.

We are thus investigating probably the simplest model which contains most of the relevant physical elements which may be of importance in the exchange couplings which lead to ferromagnetism and antiferromagnetism in d -band metals. We would hope, therefore, to find behavior corresponding to the three exchange mechanisms which have been seriously proposed for these metals: "direct" exchange between atomic d functions, Zener indirect exchange⁸ due to mobile d electrons (or, more rigorously, mobile *magnetic* electrons), and indirect exchange via " s " electrons. We do in fact find mechanisms closely similar to those of these. The first we find to be antiferromagnetic as in insulators, the second ferromagnetic but present only in special circumstances, and the third we do not investigate in detail but it seems it may be relatively small.

Van Vleck⁹ has suggested a model for magnetic transition metals in which the d electrons are partially itinerant. He pointed out that one would not expect these electrons themselves to form a band because the separations between different ionization states of the d shell are too large. In a metal the d electrons could however show an itinerant behavior because of the possibility of transferring electrons to s states. For example, one would expect the configurations $3d^{10}$ and $3d^9 4s$ but not $3d^8$ to be important in the conduction band of Ni. Virtual magnetic states describe a similar type of behavior for isolated impurities. This is another reason why it seemed of interest to investigate the magnetic interactions between such states.

Our model and techniques are essentially those of Anderson.² We assume a Hamiltonian

$$\mathcal{H} = \mathcal{H}_f + \mathcal{H}_d + \mathcal{H}_{fd}, \quad (1)$$

where

$$\mathcal{H}_f = \sum_{\mathbf{k}, \sigma} E_{\mathbf{k}} n_{\mathbf{k}}^{\sigma} \quad (2)$$

is the free (s) electron Hamiltonian and $E_{\mathbf{k}}$ and $n_{\mathbf{k}}$ are the energy and number operator for an electron with momentum \mathbf{k} in spin state σ .

$$\begin{aligned} \mathcal{H}_d = E_0 \sum_{\sigma} (n_1^{\sigma} + n_2^{\sigma}) + U (n_1^{\uparrow} n_1^{\downarrow} + n_2^{\uparrow} n_2^{\downarrow}) \\ + \sum_{\sigma} (V_{12} c_1^{\sigma*} c_2^{\sigma} + V_{21} c_2^{\sigma*} c_1^{\sigma}), \quad (3) \end{aligned}$$

where E_0 is the self-energy of the localized states (1) and (2) in the absence of interactions, U is the Coulomb

⁸ C. Zener, Phys. Rev. **91**, 303 (1953).

⁹ J. H. Van Vleck, Rev. Mod. Phys. **25**, 223 (1953); see also P. W. Anderson, Oxford discussion on magnetism, 1959 (unpublished).

repulsion between two electrons in a localized state, and

$$V_{12} = V_{21}^* = \int \varphi_1^*(\mathbf{r}) \varphi_2(\mathbf{r}) \mathcal{H}_d d\mathbf{r} \quad (4)$$

is the transfer integral between the two d states. c_i , c_i^* are, respectively, the annihilation and creation operators for a d electron at site i with spin σ , and n_i^{σ} is the corresponding number operator. Finally,

$$\mathcal{H}_{fd} = \sum_{i\mathbf{k}, \sigma} (V_{i\mathbf{k}} c_{i\mathbf{k}}^{\sigma*} c_{i\mathbf{k}}^{\sigma} + V_{i\mathbf{k}} c_i^{\sigma*} c_{\mathbf{k}}^{\sigma}) \quad (5)$$

describes the interaction of the d states with the band. Clearly

$$V_{1\mathbf{k}} = e^{i\mathbf{k} \cdot \mathbf{r}_{12}} V_{2\mathbf{k}}, \quad (6)$$

with a proper choice of phases.

To calculate the magnetic interactions we use the Green's function formalism described by Anderson² within the Hartree-Fock self-consistency scheme. The position of the Fermi level is taken as a fixed parameter which does not depend on the position of the virtual states. One obtains a set of four simultaneous equations connecting the four occupation numbers n_i^{σ} . These equations may have several stable isolated solutions so that an explicit energy calculation is necessary to determine the self-consistent state of lowest energy. In particular when both impurity sites are magnetic in themselves and V_{12} is small, the localized moments could be aligned either parallel to each other or antiparallel.

Clearly there are two types of coupling mechanism: a direct coupling due to V_{12} Eq. (3), and an indirect effect via the s - d interaction Eq. (5). The effect of the latter is oscillating and has the general character of the Ruderman-Kittel-Yosida¹⁰ interaction between localized moments.

The effect of the direct terms can be studied much more easily and has some interesting features. The sign of the effective interaction between the magnetic moment depends on the position of the virtual levels. When the virtual levels are approximately symmetrical around the Fermi level one has essentially an antiferromagnetic kinetic interaction of order V_{12}^2/U , very similar to that existing in antiferromagnetic insulators.^{8,11} On the other hand, when one of the two (single impurity) virtual levels is much closer to the Fermi surface than the other one, a parallel alignment is favored.¹² This may indicate a tendency for forming ferromagnetic bands of the VanVleck type.

¹⁰ M. A. Ruderman and C. Kittel, Phys. Rev. **96**, 99 (1954); T. Kasuya, Progr. Theoret. Phys. (Kyoto) **16**, 45 (1956); K. Yosida, Phys. Rev. **106**, 893 (1957).

¹¹ P. W. Anderson, Phys. Rev. **115**, 2 (1959).

¹² It is interesting to note that the Fermi level in a metal should tend to adjust itself to such a position because of the large d -state density.

II. THE GREEN'S FUNCTIONS

The Green's function $G(\epsilon)$ is defined by the matrix equation

$$\lim_{s \rightarrow 0} (\epsilon + is - \mathcal{H}G(\epsilon)) = 1. \quad (7)$$

As discussed by Anderson,² many properties of interest can be calculated from the density of states

$$\rho(\epsilon) = -1/\pi \operatorname{Im}(\operatorname{Tr}G(\epsilon)). \quad (8)$$

In particular the density of states in the localized states at sites 1 and 2 and of the free electrons can be found from the diagonal elements of G . Thus, e.g., for the density of states of electrons with spin σ in state 1 one has the equations:

$$(\epsilon + is - E_0 - U n_1^{-\sigma}) G_{11}^{\sigma} - V_{12} G_{21}^{\sigma} - \sum_{\mathbf{k}} V_{1\mathbf{k}} G_{\mathbf{k}1}^{\sigma} = 1, \quad (9a)$$

$$(\epsilon + is - E_0 - U n_2^{-\sigma}) G_{21}^{\sigma} - V_{21} G_{11}^{\sigma} - \sum_{\mathbf{k}} V_{2\mathbf{k}} G_{\mathbf{k}1}^{\sigma} = 0, \quad (9b)$$

$$(\epsilon + is - E_{\mathbf{k}}) G_{\mathbf{k}1}^{\sigma} - V_{\mathbf{k}2} G_{21}^{\sigma} - V_{\mathbf{k}1} G_{11}^{\sigma} = 0. \quad (9c)$$

Replacing the number operators n_i^{σ} by c numbers, the equations can be solved for G_{11}^{σ} :

$$G_{11}^{\sigma}(\epsilon) = \left[\epsilon - \epsilon_1^{\sigma} + i\Delta - \frac{(\lambda_{12} + V_{12})(\lambda_{21} + V_{21})}{\epsilon - \epsilon_2^{\sigma} + i\Delta} \right]^{-1}, \quad (10)$$

The free-electron Green's function is (again using the same phase convention)

$$G_{\mathbf{k}\mathbf{k}}^{\sigma}(\epsilon) = [(G_{\mathbf{k}\mathbf{k}}^{\sigma}(\epsilon))^0 + [G_{11}^{\sigma}(\epsilon) + G_{22}^{\sigma}(\epsilon)] \lim_{s \rightarrow 0} |V_{i\mathbf{k}}|^2 / (\epsilon + is - E_{\mathbf{k}})^2 + \lim_{s \rightarrow 0} \frac{(V_{1\mathbf{k}} V_{\mathbf{k}2} + V_{2\mathbf{k}} V_{\mathbf{k}1}) [\lambda(\epsilon) + V_{12}]}{(\epsilon - E_{\mathbf{k}} + is)^2 [(\epsilon - \epsilon_1^{\sigma} + i\Delta)(\epsilon - \epsilon_2^{\sigma} + i\Delta) - (\lambda + V_{12})^2]}, \quad (17)$$

where $(G_{\mathbf{k}\mathbf{k}}^{\sigma})^0 = \lim_{s \rightarrow 0} (\epsilon - \epsilon_{\mathbf{k}} + is)^{-1}$ is the unperturbed free-electron Green's function. The physically interesting quantity is of course the total free-electron density:

$$\begin{aligned} \rho_f^{\sigma}(\epsilon) &= -\frac{1}{\pi} \operatorname{Im} \sum_{\mathbf{k}} G_{\mathbf{k}\mathbf{k}}^{\sigma}(\epsilon) \\ &= \rho_u^{\sigma}(\epsilon) + \delta_1 \rho^{\sigma}(\epsilon) + \delta_2 \rho^{\sigma}(\epsilon). \end{aligned} \quad (18)$$

In (18),

$$\delta_1 \rho^{\sigma}(\epsilon) = \frac{\operatorname{Im}}{\pi} [G_{11}^{\sigma}(\epsilon) + G_{22}^{\sigma}(\epsilon)] \frac{d}{d\epsilon} \left[\lim_{s \rightarrow 0} \sum_{\mathbf{k}} \frac{|V_{1\mathbf{k}}|^2}{(\epsilon - E_{\mathbf{k}} + is)} \right] \quad (19a)$$

and

$$\delta_2 \rho^{\sigma}(\epsilon) = -\frac{\operatorname{Im}}{\pi} \lim_{s \rightarrow 0} \sum_{\mathbf{k}} \frac{(\lambda + V_{21}) 2 \operatorname{Re}(V_{2\mathbf{k}} V_{\mathbf{k}1})}{(\epsilon - E_{\mathbf{k}} + is)^2} \Big/ [(\epsilon - \epsilon_1^{\sigma} + i\Delta)(\epsilon - \epsilon_2^{\sigma} + i\Delta) - (\lambda + V_{12})^2]. \quad (19b)$$

where

$$\begin{aligned} \epsilon_1^{\sigma} &= E_0 + \operatorname{Re} \left(\lim_{s \rightarrow 0} \sum_{\mathbf{k}} \frac{|V_{1\mathbf{k}}|^2}{\epsilon + is - E_{\mathbf{k}}} \right) + U \langle n_1^{-\sigma} \rangle \\ &= E_0' + U \langle n_1^{-\sigma} \rangle, \end{aligned} \quad (11)$$

$$\begin{aligned} \epsilon_2^{\sigma} &= E_0' + U \langle n_2^{-\sigma} \rangle, \\ \lambda_{ij} &= \sum_{\mathbf{k}} \frac{V_{i\mathbf{k}} V_{\mathbf{k}j}}{\epsilon + is - E_{\mathbf{k}}}, \end{aligned} \quad (12)$$

$$\Delta = \Delta(\epsilon) = \operatorname{Im} \left(\lim_{s \rightarrow 0} \sum_{\mathbf{k}} \frac{|V_{1\mathbf{k}}|^2}{\epsilon + is - E_{\mathbf{k}}} \right). \quad (13)$$

For simplicity we assume the $|V_{i\mathbf{k}}|$ depends on the energy ($E_{\mathbf{k}}$) only, and that $|V_{i\mathbf{k}}|$ and the unperturbed density of states of the free electrons $[\rho_u(E)]$ are slowly varying functions of E . One then has $E_0' \approx E_0$ in Eq. (11) and

$$\Delta(\epsilon) = 4\pi^2 |V_{i\mathbf{k}}|^2 \rho_u(\epsilon), \quad (14)$$

$$\lambda(\epsilon) = \lambda_{12} = \lambda_{21} = -i\Delta(\epsilon) \sin(kr_{12}) / kr_{12} \quad (15)$$

from (12) and (13). Here k is defined by $E_{\mathbf{k}} = \epsilon$. The expression (15) for λ is clearly meaningful only in the dilute case, i.e., when r_{12} is sufficiently large, so that

$$kr_{12} \gg 1 \quad (16)$$

is the region of interest. (For the *indirect* effect only, of course.) In general, if the phases are chosen so that V_{12} is real, $\lambda_{12} = \lambda_{21}$.

The expression for $G_{22}^{\sigma}(\epsilon)$ is exactly analogous to Eq. (10).

With our previous approximations (19) becomes

$$\delta_{1\rho}{}^\sigma(\epsilon) = \frac{\text{Re}}{\pi} (G_{11}{}^\sigma(\epsilon) + G_{22}{}^\sigma(\epsilon)) \frac{d\Delta(\epsilon)}{d\epsilon}, \quad (20a)$$

$$\delta_{2\rho}{}^\sigma(\epsilon) = \frac{\text{Im}}{\pi} 2(\lambda + V_{12}) \frac{d\lambda}{d\epsilon} \Big/ [(\epsilon - \epsilon_1{}^\sigma + i\Delta)(\epsilon - \epsilon_2{}^\sigma + i\Delta) - (\lambda + V_{12})^2]. \quad (20b)$$

The first correction term $\delta_{1\rho}$ [or the corresponding term in (17)] describes the independent polarization of the free electrons by the two impurity sites. This effect is discussed in detail by Anderson (see Sec. VI of Ref. 2) and is probably small. The effect of the interference term $\delta_{2\rho}$ should be even smaller as long as (16) applies.

III. SELF-CONSISTENCY CONDITIONS

Equation (10) determines the density of states in terms of the four occupation numbers $n_i{}^\sigma$. To find a self-consistent solution one has to solve the four simultaneous equations for the $n_i{}^\sigma$

$$n_i{}^\sigma = -\frac{1}{\pi} \text{Im} \int^{\epsilon_f} G_{ii}{}^\sigma(\epsilon) d\epsilon, \quad (21)$$

where the integrals are from the bottom of the (free-electron) conduction band to the Fermi level (ϵ_f). For simplicity we assume a low concentration of localized states so that the Fermi level can be regarded as a fixed parameter which does not depend on the position of the virtual levels. Moreover we will restrict ourselves to a situation where the interactions are dominated by the transfer integral:

$$V = V_{12} \gg |\lambda(\epsilon)| \quad (22)$$

in the region of interest. One can then write [instead of (10)]:

$$\begin{aligned} G_{11}{}^\sigma(\epsilon) &= [\epsilon - \epsilon_1{}^\sigma + i\Delta - V^2/(\epsilon - \epsilon_2{}^\sigma + i\Delta)]^{-1}, \\ G_{22}{}^\sigma(\epsilon) &= [\epsilon - \epsilon_2{}^\sigma + i\Delta - V^2/(\epsilon - \epsilon_1{}^\sigma + i\Delta)]^{-1}. \end{aligned} \quad (23)$$

Equation (23) can be rewritten as

$$G_{11}{}^\sigma(\epsilon) = \frac{1}{2} [(1 + Ud^{-\sigma}/V^{-\sigma})(\epsilon - \epsilon_+{}^\sigma + i\Delta)^{-1} + (1 - Ud^{-\sigma}/V^{-\sigma})(\epsilon - \epsilon_-{}^\sigma + i\Delta)^{-1}], \quad (24)$$

$$G_{22}{}^\sigma(\epsilon) = \frac{1}{2} [(1 - Ud^{-\sigma}/V^{-\sigma})(\epsilon - \epsilon_+{}^\sigma + i\Delta)^{-1} + (1 + Ud^{-\sigma}/V^{-\sigma})(\epsilon - \epsilon_-{}^\sigma + i\Delta)^{-1}],$$

where we have defined

$$\epsilon_{\pm}{}^\sigma = E_0 + Un^{-\sigma} \pm V^{-\sigma}, \quad (25)$$

$$n^\sigma = \frac{1}{2}(n_1{}^\sigma + n_2{}^\sigma), \quad (26)$$

$$d^\sigma = \frac{1}{2}(n_1{}^\sigma - n_2{}^\sigma), \quad (27)$$

and

$$V^\sigma = +[U^2(d^\sigma)^2 + V^2]^{1/2}. \quad (28)$$

It is now convenient to replace the self-consistency conditions for the $n_i{}^\sigma$ (21) by the equivalent conditions

on the n^σ and d^σ . Clearly

$$\begin{aligned} n^\sigma &= -\frac{1}{2\pi} \text{Im} \int^{\epsilon_f} [G_{11}{}^\sigma(\epsilon) + G_{22}{}^\sigma(\epsilon)] d\epsilon \\ &= -\frac{1}{2\pi} \text{Im} \int^{\epsilon_f} [G_+{}^\sigma(\epsilon) + G_-{}^\sigma(\epsilon)] d\epsilon, \end{aligned} \quad (29)$$

$$d^\sigma = -\frac{Ud^{-\sigma}}{2\pi V^{-\sigma}} \text{Im} \int^{\epsilon_f} [G_+{}^\sigma(\epsilon) - G_-{}^\sigma(\epsilon)] d\epsilon, \quad (30)$$

where

$$G_{\pm}{}^\sigma(\epsilon) = (\epsilon - \epsilon_{\pm}{}^\sigma + i\Delta)^{-1} \quad (31)$$

from Eqs. (21) and (24) and the definitions of n^σ and d^σ . Evaluating the integrals one finally finds

$$n^\sigma = \frac{1}{2} + \frac{1}{2\pi} \left(\tan^{-1} \frac{\epsilon_f - \epsilon_+{}^\sigma}{\Delta} + \tan^{-1} \frac{\epsilon_f - \epsilon_-{}^\sigma}{\Delta} \right), \quad (32a)$$

$$d^\sigma = \frac{Ud^{-\sigma}}{2\pi V^{-\sigma}} \left(\tan^{-1} \frac{\epsilon_f - \epsilon_+{}^\sigma}{\Delta} - \tan^{-1} \frac{\epsilon_f - \epsilon_-{}^\sigma}{\Delta} \right). \quad (32b)$$

All the \tan^{-1} functions are in the range $-\frac{1}{2}\pi < \tan^{-1} < \frac{1}{2}\pi$.

One notes that there are two obvious types of solutions. Equation (32b) has the trivial solution

$$d^\dagger = d^\ddagger = 0, \quad (33)$$

which implies

$$V^\dagger = V^\ddagger = V \quad (34)$$

in Eq. (32a). These solutions describe a state where the two localized moments are parallel to each other, i.e., [from (33)]:

$$n_1{}^\sigma = n_2{}^\sigma = n^\sigma.$$

Substituting (34) in (32) one finally gets two equations for n^\dagger and n^\ddagger :

$$\begin{aligned} n^\dagger &= \frac{1}{2} + \frac{1}{2\pi} \{ \tan^{-1} [y(x - n^\dagger)^\dagger - v] \\ &\quad + \tan^{-1} [y(x - n^\ddagger)^\dagger + v] \}, \end{aligned} \quad (35)$$

$$\begin{aligned} n^\ddagger &= \frac{1}{2} + \frac{1}{2\pi} [\tan^{-1} (y(x - n^\dagger)^\ddagger - v) \\ &\quad + \tan^{-1} (y(x - n^\dagger)^\ddagger + v)], \end{aligned}$$

where we have introduced the dimensionless parameters

$$x = (E_f - E_0)/U; \quad y = U/\Delta; \quad v = V/\Delta. \quad (36)$$

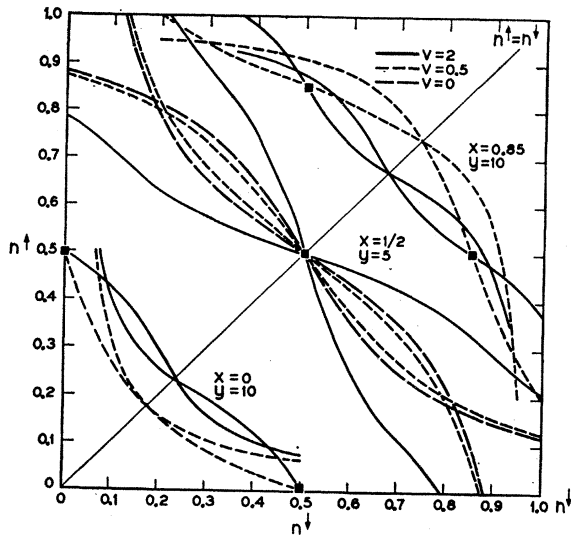


FIG. 1. Plot of $n^\uparrow(n^\downarrow)$ and $n^\uparrow(n^\uparrow)$ in the n^\uparrow, n^\downarrow plane for the following values of $x = E_f - E_0/U$, $v = V/\Delta$, and $y = U/\Delta$: (a) For $x = \frac{1}{2}$, $y = 5$ curves with $v = 0, 0.5$ and 2 are shown. Note that for $v = 2$ there is no magnetic solution; (b) $x = 0.85$, $y = 10$, $v = 0.5, 2$; (c) $x = 0$, $y = 10$, $v = 0.5, 2$. The latter value of v gives a magnetic solution. The line of nonmagnetic solutions is also shown and the points $(x, \frac{1}{2})$ and $(\frac{1}{2}, x)$ are marked by squares.

In Fig. 1 we have plotted these two functions in the n^\uparrow, n^\downarrow plane for a few values of x, y , and v .

For the second type of solution $d^\sigma \neq 0$. It follows from (32b) that:

$$d^\uparrow/d^\downarrow < 0, \quad (37)$$

so that in a sense all these solutions show a tendency for antiparallel alignment. The simple antiparallel solution for which

$$n^\uparrow = n^\downarrow = n \quad d^\uparrow = -d^\downarrow = d \quad (38)$$

is singled out by the fact that it goes to the proper limit of two antiparallel localized moments of equal magnitude as $V/U \rightarrow 0$. The model we are using is certainly meaningful only as long as V/U is small so that one feels reasonably safe in considering only these special solutions.

It follows from (38) that

$$V^\uparrow = V^\downarrow = [U^2 d^2 + V^2]^{1/2} = Uw. \quad (39)$$

(This defines w .) Using this and (38) in (32) one finds the two self-consistent equations for antiparallel moments:

$$\begin{aligned} n+w &= \frac{1}{2} + 1/\pi \tan^{-1} y(x-n+w), \\ n-w &= \frac{1}{2} + 1/\pi \tan^{-1} y(x-n-w). \end{aligned} \quad (40)$$

The existence of self-consistent magnetic solutions of either type obviously depends on the parameters in Eqs. (35) and (40). It is interesting to investigate the conditions on the parameters and in particular to see how the interaction affects the requirements (on x and y)

for the existence of localized magnetic states. We will return to this problem in Sec. V.

As one would expect intuitively the effect of the interaction on the size of the moments is usually small (when $V/U \ll 1$) except very near the critical boundary for the existence of magnetism. Over most of the range of values of x and y for which a single ion is magnetic both Eqs. (35) and (40) have stable magnetic solutions. To determine the preferred orientations (i.e., the signs of the effective magnetic interaction) one has to compare the energies.

IV. INTERACTION ENERGIES OF LOCALIZED MOMENTS

The energy of the two magnetic ions is

$$E(V) = -\frac{\text{Im}}{\pi} \int^{\epsilon_f} d\epsilon \epsilon (G_{11}^\uparrow(\epsilon) + G_{22}^\uparrow(\epsilon) + G_{11}^\downarrow(\epsilon) + G_{22}^\downarrow(\epsilon)) - U(n_1^\uparrow n_1^\downarrow + n_2^\uparrow n_2^\downarrow), \quad (41)$$

where the last term is needed because the interaction energies are counted twice in the integral. Again we neglect the polarization of the "free" electrons. Using (24), Eq. (41) can be rewritten as

$$E(V) = -\frac{\text{Im}}{\pi} \int^{\epsilon_f} d\epsilon \epsilon [G_+^\uparrow(\epsilon) + G_-^\uparrow(\epsilon) + G_+^\downarrow(\epsilon) + G_-^\downarrow(\epsilon)] - 2U(n^\uparrow n^\downarrow + d^\uparrow d^\downarrow), \quad (42)$$

where the $G_\pm(\epsilon)$ are defined in (31).

The energy in (42) depends on V through the $\epsilon_\pm^\sigma, n^\sigma$ and d^σ . Let

$$\delta\epsilon_\pm^\sigma = \epsilon_\pm^\sigma(V) - \epsilon_\pm^\sigma(0) = U\delta n^\sigma \pm \delta V^{-\sigma}, \quad (43)$$

$$\begin{aligned} \delta n^\sigma &= n^\sigma(V) - n^\sigma(0); \quad \delta d^\sigma = d^\sigma(V) - d^\sigma(0); \\ \delta V^\sigma &= V^\sigma(V) - V^\sigma(0) = V^\sigma(V) - Ud^\sigma(0). \end{aligned} \quad (44)$$

The change in energy due to introducing V is, then, to second order in the δ 's

$$\begin{aligned} E(V) - E(0) &= \sum_\sigma \{ \delta\epsilon_+^\sigma n_+^\sigma(0) + \delta\epsilon_-^\sigma n_-^\sigma(0) \\ &\quad - \frac{1}{2} [(\delta\epsilon_+^\sigma)^2 \rho_+^\sigma(0) + (\delta\epsilon_-^\sigma)^2 \rho_-^\sigma(0)] \} \\ &\quad - 2U [n^\uparrow(0)\delta n^\downarrow + n^\downarrow(0)\delta n^\uparrow + d(0)^\uparrow \delta d^\downarrow \\ &\quad + d(0)^\downarrow \delta d^\uparrow + \delta n^\uparrow \delta n^\downarrow + \delta d^\uparrow \delta d^\downarrow], \end{aligned} \quad (45)$$

where

$$n_\pm^\sigma(V) = \frac{1}{2} + 1/\pi \tan^{-1} [\epsilon_f - \epsilon_\pm^\sigma(V)]/\Delta \quad (46)$$

and

$$\rho_\pm^\sigma(V) = (1/\pi)\Delta / [(\epsilon_f - \epsilon_\pm^\sigma(V))^2 + \Delta^2] \quad (47)$$

are the occupation number and density of states for the virtual states described by the $G_\pm(\epsilon)$ (31). The meaning of (45) is fairly obvious (see Figs. 2 and 3). The first two terms describe the energy change of the four virtual levels when shifted by a small amount so that terms of order

$$(\delta\epsilon)^3 (d\rho/d\epsilon) \quad (48)$$

can be neglected.

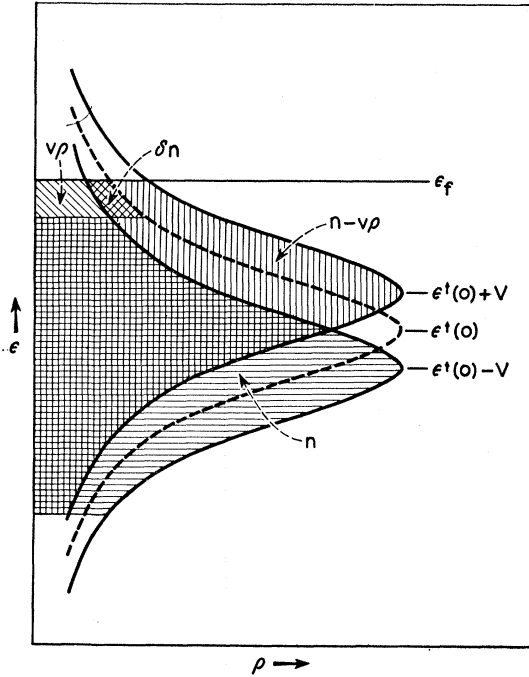


FIG. 2. Schematic diagram showing change in energy for parallel spins. Without interaction the virtual levels at both sites are at $\epsilon^\dagger(0)$ and each contains n electrons. The splitting by V shifts n electrons down and $n - V\rho$ electrons up (by V). The slice $V\rho$ near ϵ_f remains unchanged. The change in energy is therefore $V^2\rho$.

When the two moments are parallel to each other, one has

$$n_+^\sigma(0) = n_-^\sigma(0) \quad V^\sigma = \delta V^\sigma = V \quad d^\sigma = \delta d^\sigma = 0, \quad (49)$$

so that (45) becomes

$$[E(V) - E(0)]_{\text{par}} = -(U^2 \delta n^{\uparrow 2} + V^2) \rho^\dagger(0) - (U^2 \delta n^{\downarrow 2} + V^2) \rho^\dagger(0) - 2U \delta n^\dagger \delta n^\dagger. \quad (50)$$

For sufficiently small δn this reduces to

$$[E(V) - E(0)]_{\text{par}} = -V^2(\rho^\dagger + \rho^\dagger). \quad (51)$$

This is illustrated in Fig. 2. To see if this is consistent one has to check whether

$$U^2 \delta n^2 \ll V^2, \quad (52)$$

and, moreover,

$$U \delta n^\dagger \delta n^\dagger \ll V^2(\rho^\dagger + \rho^\dagger). \quad (53)$$

The last requirement is particularly important because δn^\dagger and δn^\dagger have opposite signs in the magnetic state and the last term on the right-hand side of (50) is therefore positive.

From (35) one finds

$$\begin{aligned} \delta n^\dagger &= -U \delta n^\dagger \rho^\dagger + \frac{1}{2}(U^2 \delta n^{\uparrow 2} + V^2)(d\rho^\dagger/d\epsilon), \\ \delta n^\dagger &= -U \delta n^\dagger \rho^\dagger + \frac{1}{2}(U^2 \delta n^{\downarrow 2} + V^2)(d\rho^\dagger/d\epsilon). \end{aligned} \quad (54)$$

Clearly δn is at most of order V^2 but one has to check whether $U \delta n$ is still small.

In a properly magnetic state ($|n^\dagger - n^\dagger| \sim 1$) at least one of the virtual states is far from the Fermi surface. We assume also:

$$V/U, \quad \Delta/U \ll 1. \quad (55)$$

Consider first a symmetric situation:

$$(\epsilon_f - E_0)/U \sim \frac{1}{2}. \quad (56)$$

Then

$$U \rho^\dagger \sim U \rho^\dagger \sim \Delta/U \ll 1 \quad (57)$$

and

$$d\rho/d\epsilon \sim \Delta/U^3. \quad (58)$$

It follows that

$$|U \delta n| \sim V^2 \Delta/U, \quad (59)$$

and both (52) and (53) hold. The energy gain (51) becomes

$$E(V) - E(0) \approx -8V^2 \Delta/\pi U^2. \quad (60)$$

In an asymmetric situation

$$(\epsilon_f - E_0)/U \sim 0 \quad \text{or} \quad 1 - (\epsilon_f - E_0)/U \sim 0; \quad (61)$$

one virtual state (e.g., ϵ^\dagger) is much nearer to ϵ_f than the second one, i.e.,

$$\left| \frac{\epsilon_f - \epsilon^\dagger}{\epsilon_f - \epsilon^\dagger} \right| \sim \frac{\epsilon_f - \epsilon^\dagger}{U} \ll 1. \quad (62)$$

A sufficient condition for the expansion is now:

$$V/|\epsilon_f - \epsilon^\dagger| \ll 1. \quad (63)$$

From (54), (55), and (63)

$$\delta n^\dagger \sim -(\Delta/\pi U) \delta n^\dagger \ll \delta n^\dagger \quad (64)$$

so that

$$\delta n^\dagger \approx \frac{1}{2} V^2 \frac{d\rho^\dagger}{d\epsilon} / \left(1 - \frac{\Delta}{\pi} \rho^\dagger \right) \sim V^2 / (\epsilon_f - \epsilon^\dagger)^2. \quad (65)$$

From (64) and the estimate of ρ implied by (62), it follows that the corrections to the energy (50), because of changes in occupation, are at most of order $V^2 \delta n^2$. The corrections are therefore small when (63) holds.

For antiparallel moments:

$$\begin{aligned} n_+^\dagger(0) &= n_+^\dagger(0) = n_+, \\ n_1^\dagger(0) &= n_2^\dagger(0), \\ n_-^\dagger &= n_-^\dagger = n_-. \end{aligned} \quad (66)$$

The situation is illustrated in Fig. 3. Now

$$d^\dagger(0) = -d^\dagger(0) = \frac{1}{2}(n_+(0) - n_-(0)) = -d \quad (67)$$

and

$$\delta V^\dagger = \delta V^\dagger = U \delta d - V^2/2Ud. \quad (68)$$

Substituting in (45) one gets:

$$[E(V) - E(0)]_{\text{ap}} = -(2V^2/U) - U^2(\delta n + \delta d)^2 \rho_+ - U^2(\delta n - \delta d)^2 \rho_- - 2U(\delta n^2 - \delta d^2). \quad (69)$$

The terms in δn and δd can be calculated from the self-

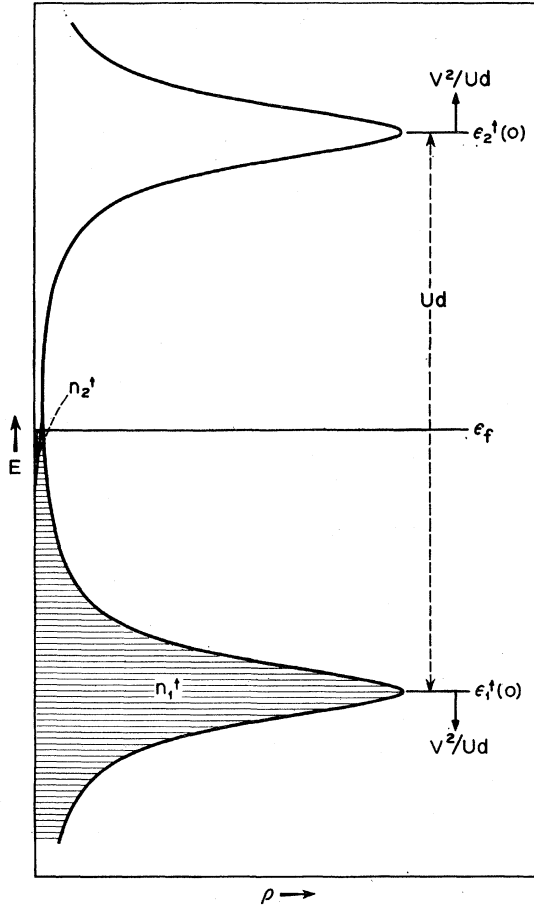


FIG. 3. Energy change for antiparallel moments.

consistency equations (40), i.e.,

$$(\delta n + \delta d) = -U(\delta n - \delta d)\rho^- + U^2 \frac{(\delta n - \delta d)^2 d \rho^-}{2 d \epsilon} - \frac{V^2}{2Ud} \rho^-, \quad (70)$$

$$(\delta n - \delta d) = -U(\delta n + \delta d)\rho^+ + \frac{U^2(\delta n + \delta d)^2 d \rho^+}{2 d \epsilon} - \frac{V^2}{2Ud} \rho^+.$$

An argument similar to that for the parallel case shows that all correction terms are small as long as

$$V/|\epsilon_f - \epsilon_{\pm}| \ll 1; \quad \Delta/U \ll 1. \quad (71)$$

Consequently,

$$[E(V) - E(0)]_{\text{ap}} \approx -2V^2/U. \quad (72)$$

This is of course just superexchange, as defined by Anderson in Ref. 13 (called "kinetic exchange" in Ref. 2).

Comparing (72) with (51) it is clear that a parallel arrangement is favored when

$$\frac{1}{2}U(\rho^{\uparrow}(0) + \rho^{\downarrow}(0)) > 1. \quad (73)$$

In a symmetric situation both virtual levels are far from ϵ_f ($\epsilon_f - \epsilon^o$) and the left-hand side of the inequality (73) is approximately Δ/U [see (57)]. It is thus clear that antiferromagnetic superexchange is favored. In fact the Lorentzian model of the virtual state certainly exaggerates the magnitude of ρ far from the center of the virtual level, which makes the argument even stronger.

For an asymmetric situation one virtual level is close to the Fermi surface and has a large density of states there, so that (73) can hold. If, in particular, the Fermi level is well within the virtual state, the left-hand side of (73) becomes of order U/Δ and therefore large.

We have seen that the sign of the magnetic coupling depends on the position of the Fermi level relative to the impurity energy E_0 . When ϵ_f is near E_0 or near $E_0 + U$ parallel spins are favored, whereas in the intermediate region one finds antiferromagnetic "superexchange." This results from a competition between two coupling mechanisms. Clearly a *single* electron, distributed among the two d states, would have the same spin direction at both sites. For exactly two electrons (and large U) it is most favorable to have opposite spins so that each electron can interact with an empty (ionized) state of proper spin. Our virtual states have nonintegral occupations and the position of the Fermi level determines which mechanism is dominant.

The ferromagnetic mechanism is very similar to the Zener double-exchange mechanism.^{13,8} It is likely that the generalization of the above criterion for ferromagnetism which will apply in more general situations is the requirement of a high density of magnetic electrons near the Fermi surface. We intend to study the more realistic case of coupling between atoms with orbitally degenerate d levels in the future.

V. THE CRITICAL BOUNDARY

The conditions for the validity of the approximations of the last section are quite stringent and one would like to know what happens near the critical boundary for magnetism when they are no longer valid.

We have seen that the state with parallel moments is favored in an asymmetric situation when one of the virtual levels is very close to the Fermi surface. This implies that these solutions are important mainly near the critical boundary. It is therefore of particular interest to investigate the stability of the solutions of (35) near the boundary for the magnetism of a single ion. This is best done by looking at the solutions of (35) on this critical boundary. We still show that (35) has no magnetic solutions on the boundary in a symmetric situation ($x \sim \frac{1}{2}$). On the other hand, in an asymmetric situation ($x \sim 0, 1$), (35) does have such solutions on the boundary and even beyond it.

Equations (35) always have a nonmagnetic solution

¹³ P. W. Anderson, Solid State Phys. 14, 99 (1963).

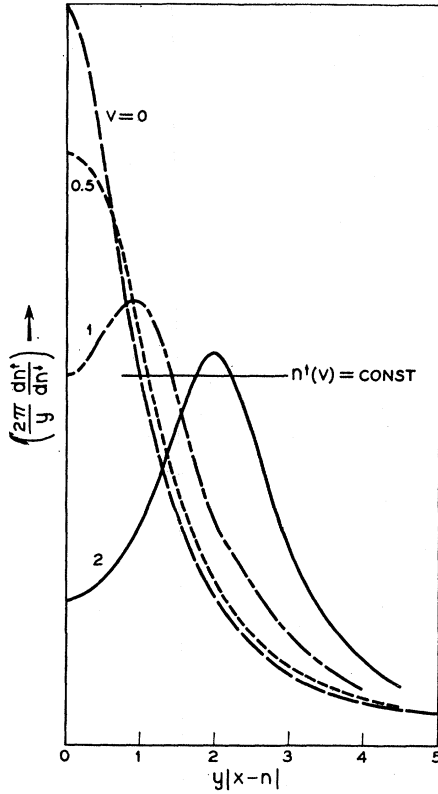


FIG. 4. The density of states $[(\xi-v)^2+1]^{-1} + [(\xi+v)^2+1]^{-1}$ for $v=0, 0.5, 1,$ and 2 as a function of $\xi=y(x-n)$. The level where $n=\text{constant}$ at constant slope is also marked.

where $n^\dagger = n^\downarrow = n(v)$. This solution becomes unstable when

$$(\partial n^\dagger / \partial n^\dagger)_{n^\dagger = n^\downarrow = n} < -1 \quad (74)$$

(see Fig. 1). This is therefore a sufficient condition for magnetism.¹⁴ Differentiating (35a) one has

$$\frac{\partial n^\dagger}{\partial n^\downarrow} = -\frac{y}{2\pi} \left\{ \frac{1}{[(y(x-n^\dagger)-v)^2+1]} + \frac{1}{[(y(x-n^\dagger)+v)^2+1]} \right\}. \quad (75)$$

The expression in curved brackets is plotted in Fig. 4 for several values of v . For the particular case $x = \frac{1}{2}$ we know that $n = \frac{1}{2}$. One then finds

$$y_c(\frac{1}{2}, v) = \pi(1+v^2), \quad (76)$$

where $y_c(x, v)$ is the value of y on the critical boundary

¹⁴ When (74) does not hold the nonmagnetic solution is stable. For small values of v this implies that there are no magnetic solutions. However, when $v^2 > \frac{1}{3}$, each of the curves (35) has three inflection points so that they can have five simultaneous solutions. There is then a limited range of x and y in which both magnetic and nonmagnetic solutions exist and are stable. This effect results from the splitting of the virtual level by v (Fig. 4) and is probably fortuitous. Clearly (74) is still a sufficient condition for magnetism and it is at least necessary that the maximum slope of $n^\dagger(n^\downarrow)$ be smaller than -1 .

where $\partial n^\dagger / \partial n^\downarrow = -1$. It is thus clear that the magnetic region is reduced in this vicinity. In fact one can fairly easily do a little better. In the Appendix it is shown that the slope of $n^\dagger(n^\downarrow)$ is decreased at the nonmagnetic solution and, therefore,

$$y_c(x, v) > y_c(x, 0) \quad (77)$$

for all values of x , such that

$$y_c(x, 0) / \pi < 4/3. \quad (78)$$

This can be interpreted as a criterion for a range of values of x for which the interaction has an unfavorable effect on the magnetic transition. Roughly this is the range

$$0.2 < x < 0.8, \quad (79)$$

as can be seen, e.g., in Fig. 5.

In the vicinity of $x=0$ and $x=1$ the slope of the curves at the nonmagnetic solution is increased. It is shown in

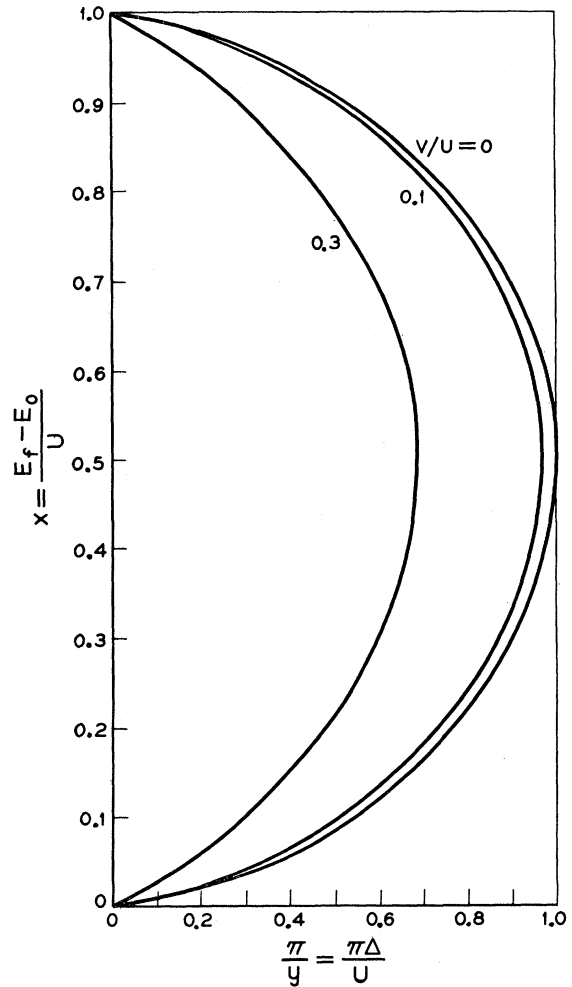


FIG. 5. Critical boundaries for the existence of antiparallel magnetic solutions for $V/U=0, 0.1$ and 0.3 . The curves were computed from Eq. (85).

the Appendix that $y_c(x, v)$ is certainly larger than $y_c(x, 0)$ when

$$y_c(x, 0)/\pi \geq 2, \quad (80)$$

i.e., when

$$x \lesssim 0.09 \quad \text{and} \quad x \gtrsim 0.91. \quad (81)$$

The transition from one region to the other takes place somewhere between the ranges (81) and (79) and is not really of interest. The numerical values of the limits in the inequalities (78)–(81) are in any case sensitive to the details of the model and cannot be taken very seriously. In particular one would expect the “favorable” regions to decrease with a more realistic shape of the virtual level.

The discussion of the antiparallel case is quite straightforward. If one considers $(n+w)$ and $(n-w)$ as variables in Eqs. (40), these equations become formally equivalent to the Anderson² equations for a single ion

$$n^\sigma = \frac{1}{2} + (1/\pi) \tan^{-1} y(x - n^{-\sigma}). \quad (82)$$

The self-consistent value of $w(w_{sc})$ calculated from (40) is therefore equal to half the magnitude of the localized moment calculated from (82):

$$|n^\uparrow(0) - n^\downarrow(0)| = 2w_{sc} \quad (83)$$

for the same values of x and y . The solutions of (40) are however meaningful only when

$$w \geq V/U = w_c \quad (84)$$

by definition (39). The actual magnetic region of (40) is thus given by these values of x , y for which (82) would give $|n^\uparrow - n^\downarrow| \geq 2V/U$ and is therefore smaller than that of a single ion. This may be connected with the relative rarity of metallic antiferromagnets. In fact it is obvious from the above arguments that the interaction always tends to decrease the size of the moments.

The critical boundary of (40) is given by setting $w = w_c$ in the equations. This gives parametric equations for x and y on the boundary in terms of n :

$$\begin{aligned} x_c &= n - (w_c/\sin 2\pi w_c) \sin 2\pi n, \\ \frac{2\pi}{y_c} &= (2\pi w_c/\sin 2\pi w_c) (\cos 2\pi w_c - \cos 2\pi n). \end{aligned} \quad (85)$$

The boundary for several values of w_c is plotted in Fig. 5.

VI. DISCUSSION

The above results are of course only a preliminary approach to a very complicated problem. Even the model itself is treated only in Hartree-Fock approximation; that this is rather primitive may be seen by realizing that the corresponding approximation for a pure magnetic metal is the Stoner-Slater free-electron theory of ferro- and antiferromagnetism. Nonetheless it appears that Hartree-Fock may be more accurate and is

certainly simpler and more transparent in the local moment model than in the pure model.

Another very serious limitation is the use of only a single nondegenerate orbital on each solute atom. It is amazing and rather gratifying that the model is nonetheless subtle enough that a Zener-like mechanism comes out. The criterion for this mechanism is transparently generalizable to the more complex case, and it will be interesting to see how this works out quantitatively.

Physically, we can see that the antiferromagnetic effect is very like “kinetic exchange,”¹³ in that it comes about because energy is to be gained by *virtual* transfer of electrons from the full spin-down level on one atom to the empty spin-down level on the other and vice versa. This, being a purely virtual process, requires no level density at the Fermi surface and so is favored by well-localized, symmetrically disposed virtual states.

The ferromagnetic effect, on the other hand, depends on an energy gain coming from real transitions of electrons of one spin back and forth between the two virtual states, and therefore works well when one state has a large density near the Fermi surface, precisely the case in which the antiferromagnetic effect is inefficient.

APPENDIX: EFFECT OF THE INTERACTION ON THE CRITICAL BOUNDARY FOR PARALLEL MOMENTS

In the parallel case we want to compare the stability region of magnetic solutions of (35) with that of (82). This can be done by investigating the derivative of (35) at the nonmagnetic solution:

$$[\partial n^\uparrow(n^\uparrow, x, y, v)/\partial n^\uparrow]_{n^\uparrow = n^\downarrow = n(v)} \quad (A1)$$

for values of x and y on the critical boundary of (82). This is sufficient to see the direction in which v moves the boundary for any value of x and y .

One first notes that

$$|x - n(v)| > |x - n(0)| \quad (A2)$$

as can be seen from (35) and (85), or e.g., in Fig. 6.

We will first investigate the conditions for a decrease in the slope. It follows from (75) that

$$|(\partial n^\uparrow/\partial n^\uparrow)(n^\uparrow, x, y, v)| < |(\partial n^\uparrow/\partial n^\uparrow)(n^\uparrow, x, y, 0)| \quad (A3)$$

when

$$y^2(x - n^\uparrow)^2 \leq (v^2 + 1/3). \quad (A4)$$

Now for small v ($v^2 < \frac{1}{3}$) $|(\partial n^\uparrow/\partial n^\uparrow)|$ is also a monotonic decreasing function of $|x - n^\uparrow|$. It then follows from (A2) and (A3) that

$$\begin{aligned} \left| \frac{\partial n^\uparrow(x, y, v)}{\partial n^\uparrow} \right|_{n^\uparrow = n(v)} &< \left| \frac{\partial n^\uparrow(x, y, v)}{\partial n^\uparrow} \right|_{n^\uparrow = n(0)} \\ &< \left| \frac{\partial n^\uparrow(x, y, 0)}{\partial n^\uparrow} \right|_{n^\uparrow = n(0)} \end{aligned} \quad (A5)$$

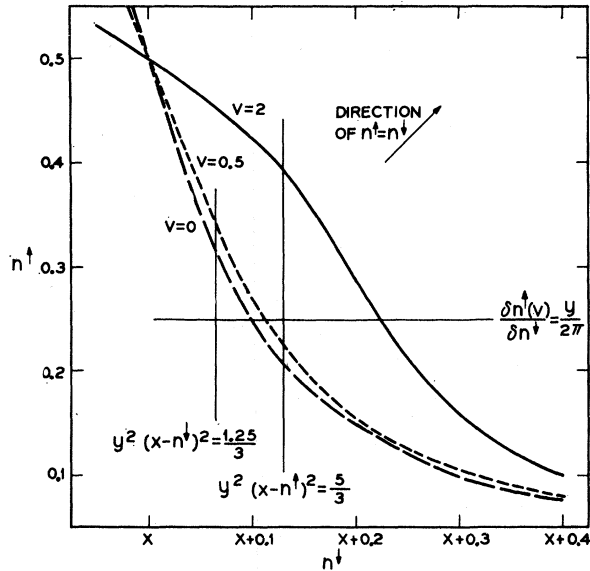


FIG. 6. Plot of

$$n^\dagger(n^\dagger) = \frac{1}{2} + (1/2\pi) [\tan^{-1}(y(x-n^\dagger)-v) + \tan^{-1}(y(x-n^\dagger)+v)]$$

for $y=10$ and $v=0, 0.5$ and 2 as a function of $x-n^\dagger$. Only the lower part of the curves ($n^\dagger < 0.5$) are shown. The places where the slope of $n^\dagger(v)$ becomes larger than that of $n^\dagger(0)$ at constant n^\dagger [the vertical lines $(x-n^\dagger)^2 = (v^2+1)/3y^2$] and at constant n [the horizontal line $\partial n^\dagger(v)/\partial n^\dagger = \text{constant}$] are shown. The position of the nonmagnetic solutions $n(v)$ depends on x . It can be seen from the direction of the line $n^\dagger = n^\dagger$ that $n^\dagger(v)$ always has a larger slope when x is such that $n(0) < \frac{1}{4}$.

when (A4) holds at $n(0)$. On the critical boundary for $v=0$ (75) becomes

$$[y_c(x,0)/\pi] - 1 = y_c^2(x,0)(x-n_c(x,0))^2. \quad (\text{A6})$$

Substituting this in (A4), it then follows that (A5) holds on the critical boundary for $v=0$, and therefore

$$y_c(x,v) > y_c(x,0) \quad (\text{A7})$$

when

$$y_c(x,0)/\pi \leq (4+v^2/3); \quad v^2 \leq \frac{1}{3}. \quad (\text{A8})$$

For large v ($v^2 > \frac{1}{3}$) the above argument no longer holds because $\partial n^\dagger/\partial n^\dagger$ has two separated maxima. The maximum of (75) is however smaller than $4\pi/3y$ for such values of v , and one has at least

$$y_c(v)/\pi > \frac{1}{3}yv^2 > \frac{1}{3}. \quad (\text{A9})$$

This is approximately equivalent to (A8) as a condition on the range of x for which (A7) holds. Roughly this is the range:

$$0.2 < x < 0.8.$$

We now want to show that there is a range of x near $x=0$ (and near $x=1$) where (35) has magnetic solutions on the critical boundary of (82) so that

$$y_c(x,v) < y_c(x,0). \quad (\text{A10})$$

For this it is sufficient to show that

$$\left| \frac{\partial n^\dagger}{\partial n^\dagger}(n^\dagger, v) \right|_{n^\dagger = n^\dagger - n(v)} > \left| \frac{\partial n^\dagger}{\partial n^\dagger}(n^\dagger, 0) \right|_{n^\dagger = n^\dagger - n(0)}. \quad (\text{A11})$$

For small v , (A11) will follow if

$$\left| \frac{\partial n^\dagger(n^\dagger, x, y, v)}{\partial n^\dagger} \right|_{n^\dagger(n^\dagger) = n(0)} > \left| \frac{\partial n^\dagger(n^\dagger, x, y, 0)}{\partial n^\dagger} \right|_{n^\dagger = n^\dagger - n(0)}, \quad (\text{A12})$$

because the left-hand side (A12) is smaller than the left-hand side of (A11) (see Fig. 6). We therefore want to compare the slope of $n(n, v)$ with that of $n(n, 0)$ when

$$(n^\dagger(n^\dagger, v))_{n^\dagger = \alpha} = (n^\dagger(n^\dagger, 0))_{n^\dagger = \beta}. \quad (\text{A13})$$

To do this it is convenient to invert (35), i.e.,

$$\tan 2\pi(n^\dagger - \frac{1}{2}) = 2y(x-n^\dagger)/[1+v^2-y^2(x-n^\dagger)^2]. \quad (\text{A14})$$

Substitution of (A13) now gives

$$\frac{x-\alpha}{x-\beta} = \frac{1+v^2-y^2(x-\alpha)^2}{1-y^2(x-\beta)^2}. \quad (\text{A15})$$

Differentiating (A14) gives

$$\frac{\pi}{\cos^2 2\pi(n^\dagger - \frac{1}{2})} \frac{\partial n^\dagger}{\partial n^\dagger} = -y \left[\frac{1}{1+v^2-y^2(x-n^\dagger)^2} + \frac{2y(x-n)}{[1+v^2-y^2(x-n^\dagger)^2]^2} \right]. \quad (\text{A16})$$

Using (A15) in (A16) it is seen that (A12) holds when

$$y^2[x-n(0)]^2 \geq 1 \quad (\text{A17})$$

and the denominator of the first term on the right-hand side of (A16) is therefore negative. On the critical boundary (for $v=0$) we can now use (A6) to get

$$y_c(x,0)/\pi \geq 2. \quad (\text{A18})$$

For large v ($v^2 > \frac{1}{3}$) (A11) does not follow from (A12). It can however be shown that (A18) is still a sufficient condition.