

The long-wavelength approximation is obtained by expanding the integrand in a power series in x and using only the lowest nonvanishing term. The result is $U=5.0$. Hence the long-wavelength approximation leads to a result which, in the limit of high temperatures, is too large by roughly a factor of 3.

Next the long-wavelength approximation is used to obtain an upper estimate on the error due to the high-temperature approximation. If one drops constant factors and replaces $\hbar\omega/kT$ by y , the relevant integral becomes

$$I = T^5 \int_0^\theta y^6 (\cosh y - 1)^{-1} dy, \quad (B4)$$

where $\theta = \Theta/T$. Since the integrand satisfies the inequalities

$$y^4 \theta^2 (\cosh \theta - 1)^{-1} \leq y^6 (\cosh y - 1)^{-1} \leq 2y^4 \quad (B5)$$

in the range $0 \leq y \leq \theta$, I satisfies the inequalities

$$\frac{1}{2} \theta^2 [\cosh \theta - 1]^{-1} \leq I/I' \leq 1, \quad (B6)$$

where I' is the high-temperature limit of I , obtained by replacing the integrand of (B4) by $2y^4$. For $\theta=3$, i.e., $T=\frac{1}{3}\Theta$, (B6) shows that I' overestimates I by at most a factor of 2.

Localized Moments in Metals

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(Received July 14, 1961)

A simple model is used to study the occurrence of localized magnetic moments in dilute alloys. The phenomenon is treated as a scattering problem in which conduction electrons scatter from impurity potentials. Under appropriate circumstances the scattering amplitude may show a resonance—corresponding to a virtual level of the impurity. It is shown that if such a level is sufficiently sharp and lies close enough to the Fermi level, the impurity atom will develop an exchange potential that polarizes neighboring electrons. The potentials for spin-up and spin-down electrons are determined by a pair of coupled equations, whose solutions are discussed in a number of interesting cases.

I. INTRODUCTION

IN recent publications Matthias, *et al.*¹ have discussed the remarkable behavior of dilute ($\sim 1\%$) solutions of Fe in various $4d$ elements and alloys. From susceptibility measurements they demonstrate that in certain of these solvents the Fe atoms possess a localized magnetic moment, whereas in others they do not. Study of a wide variety of such alloys leads them to a plot of the magnitude of the localized moment versus atomic number in the $4d$ series that shows three maxima—one at the beginning of the series, one in the vicinity of Mo, and one near Rh and Pd—separated by regions in which the Fe atoms are unpolarized. Anderson,² following the ideas of Friedel,³ has proposed a simple model to explain this behavior. He considers a localized level (representing a d state of the Fe atom) immersed in a sea of mobile electrons (representing the band of the $4d$ element or alloy). The one-electron portion of the Hamiltonian is chosen to include the energies of the localized and running wave (Bloch) states, as well as off-diagonal matrix elements that couple the two. It is

also assumed that there is a Coulomb energy of the form $Un_{d\uparrow}n_{d\downarrow}$, where $n_{d\uparrow}$ and $n_{d\downarrow}$ are the number of electrons with spin up and spin down in the localized level. In this model the coupling between the Bloch waves and the localized state broadens the latter—making it into a virtual level of the type discussed by Friedel. Whether or not this virtual level carries a moment is then determined by its position and width in comparison to the Coulomb energy. If it lies close to the Fermi level and is narrow (compared to U) it will be split by the Coulomb interaction and thus polarize, but in other cases it remains unmagnetized. Thus one has a picture in which the occurrence of a localized moment depends sensitively on the position and width (which is proportional to the density of states) of the virtual level. By assuming that these quantities vary smoothly throughout the $4d$ series, it is then possible, in a qualitative way, to understand the behavior of the Fe moment.

In this paper we wish to consider the problem of the localized moments—again using an exceedingly simple model—from a somewhat different point of view. We consider it as a scattering problem in which the conduction electrons of the $4d$ elements scatter from the potential due to a (single) iron impurity atom. In this language (see Friedel), the virtual level manifests itself as a maximum in the impurity scattering cross section

¹ B. T. Matthias, M. Peter, H. J. Williams, A. M. Clogston, E. Corenzwit, and R. C. Sherwood, *Phys. Rev. Letters* **5**, 542 (1960). A. M. Clogston, B. T. Matthias, M. Peter, H. J. Williams, E. Corenzwit, and R. C. Sherwood (to be published).

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

³ J. Friedel, *Suppl. Nuovo cimento* **7**, 287 (1958).

as a function of the energy of the incoming electron. We then show—in a self-consistent way within the framework of the Hartree-Fock theory—that if this virtual level is sufficiently sharp and close enough to the Fermi level, the Fe atom will develop an exchange potential that polarizes the electrons in its vicinity. The most important matrix element of this exchange potential corresponds to the interaction $Un_{d\uparrow}n_{d\downarrow}$ postulated by Anderson. It is not surprising, therefore, that the results predicted by our model are very similar to his. The point of view and starting approximations are, however, sufficiently different that it seems worthwhile to describe them in some detail. In particular, our formulation makes very clear the role of the Coulomb and exchange energies that split the virtual level, and thus give rise to localized moments.

II

In the following we will be concerned with the scattering of Bloch waves from a single substitutional impurity atom in an otherwise perfect crystal. Throughout we will assume that the wave functions may be expanded in terms of Wannier functions from a *single band*—that is, we shall neglect interband matrix elements of the impurity potential, V . We shall also assume that the only in-band matrix element of V is the diagonal one connecting two Wannier functions localized at the impurity. These (admittedly drastic) assumptions are the same as those made by Koster and Slater⁴ in their treatment (for a different purpose) of the impurity problem, and make possible the rather simple manipulations which follow.

The Schrödinger equation that determines the scattering wave functions may be written in the form⁵

$$\psi = \varphi_{\mathbf{k},m} + \left\{ \frac{1}{[E_m(\mathbf{k}) - H_0 + is]} \right\} V\psi, \quad (1)$$

where $\varphi_{\mathbf{k},m}$ is the incoming Bloch wave, of wave vector \mathbf{k} , in band m , having energy $E_m(\mathbf{k})$ (henceforth, we abbreviate this as E); H_0 is the one-electron Hamiltonian (including the Hartree-Fock field) of the unperturbed problem; and V is the potential of the impurity atom. If $a_m(\mathbf{r} - \mathbf{R}_i)$ is the Wannier function for band m , centered at position \mathbf{R}_i , our previous assumption tells us that the matrix elements of V satisfy the relation

$$(a_n(\mathbf{r} - \mathbf{R}_i), Va_{n'}(\mathbf{r} - \mathbf{R}_j)) = V_{nn'}\delta_{nn'}\delta(\mathbf{R}_i - \mathbf{R}_0)\delta(\mathbf{R}_j - \mathbf{R}_0), \quad (2)$$

where \mathbf{R}_0 is the location of the impurity. With this approximation for V it is now a straightforward matter, using the methods of Koster and Slater, to solve Eq. (1). If we write

$$\psi = \sum \mathbf{R}_i [U_m(\mathbf{R}_i) a_m(\mathbf{r} - \mathbf{R}_i)], \quad (3)$$

⁴ G. F. Koster and J. C. Slater, Phys. Rev. **96**, 1208 (1954).

⁵ G. F. Koster, Phys. Rev. **95**, 1436 (1954).

we find that $U_n(\mathbf{R}_i)$ is determined by the relation

$$U_n(\mathbf{R}_i) = \delta_{nm} e^{i\mathbf{k} \cdot \mathbf{R}_i} + \sum_{\mathbf{k}'} \left\{ \frac{\exp[i\mathbf{k}' \cdot (\mathbf{R}_i - \mathbf{R}_0)]}{[E - E_n(\mathbf{k}') + is]} V_{nn} U_n(\mathbf{R}_0) \right\}. \quad (4)$$

In particular,

$$U_m(\mathbf{R}_0) \{1 - V_{mm} \sum_{\mathbf{k}'} [1/(E - E_m(\mathbf{k}') + is)]\} = e^{i\mathbf{k} \cdot \mathbf{R}_0}. \quad (5)$$

The integral in this equation—which has both real and imaginary parts—may be rewritten in the form

$$\begin{aligned} \int \frac{d^3k'}{(2\pi)^3} \left[\frac{1}{E - E_m(\mathbf{k}') + is} \right] &= \int \frac{\rho_m(\epsilon) d\epsilon}{[E - \epsilon + is]} \\ &= P \int \frac{\rho_m(\epsilon) d\epsilon}{(E - \epsilon)} - i\pi \rho_m(E), \end{aligned} \quad (6)$$

where $\rho_m(E)$ is the density of states in band m , and the symbol P indicates that the principal value is to be taken. We will designate this principal-value integral by the symbol

$$F_m(E) = P \int \frac{\rho_m(\epsilon) d\epsilon}{(E - \epsilon)}. \quad (7)$$

From Eq. (5) we have

$$U_m(\mathbf{R}_0) = e^{i\mathbf{k} \cdot \mathbf{R}_0} / \{ [1 - V_{mm} F_m(E)] + i\pi V_{mm} \rho_m(E) \}. \quad (8)$$

and we may compute the values of U_m at other lattice points by using this result in conjunction with Eq. (4).

We now wish to consider the factor $[1 - V_{mm} F_m(E)]$ that appears in the denominator of Eq. (8). In particular, we are interested in the zeros of this expression, which may be obtained from a plot of $F_m(E)$ vs E . As may be seen from Eq. (7), this function approaches $1/E$ for large positive or negative values of E . In the intermediate range its behavior is determined by $\rho_m(E)$ and, if the latter is a fairly smooth function, will have the general form of a dispersion curve as illustrated in Fig. 1. The zeros of the expression $[1 - V_{mm} F_m(E)]$ are then determined by the intersections of the line $(1/V_{mm})$ with $F_m(E)$. For example, in Fig. 1 we illustrate a case in which, for an attractive potential, there are two roots (labeled A and B). It is clear from the diagram that the

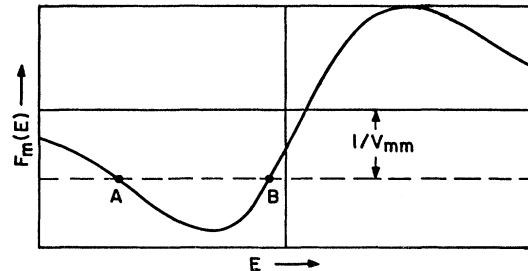


FIG. 1. Typical plot of $F_m(E)$ vs E .

roots occur in pairs and that, for the simple sort of $F_m(E)$ curve that we are considering, there can be either zero or two of them. We shall be interested in the case in which there are two roots, and will particularly focus our attention on that root of the equation

$$[1 - V_{mm}F_m(E)] = 0 \quad (9)$$

at which $F_m(E)$ has a negative derivative (root *A* of Fig. 1). It will become clear later that this root, which we shall call E_0 , is the one of interest as far as spin polarization is concerned.

Two cases may now arise. If E_0 lies outside the band in question, then $\rho_m(E_0) = 0$ and $U_m(R_0) \rightarrow \infty$ as $E \rightarrow E_0$. This case has been extensively studied by Koster and Slater. The fact that $U_m(R_0) \rightarrow \infty$ as $E \rightarrow E_0$ implies that there is a finite value of U_m with no incoming wave, i.e., that there is a bound state of the impurity atom at energy E_0 . On the other hand, if E_0 lies within the band, $\rho_m(E_0)$ is finite and $U_m(R_0)$, rather than going to infinity at $E = E_0$, merely shows a resonance there. This resonance is a virtual level of the type discussed by Friedel, and corresponds to a maximum, at that energy, of the impurity scattering cross section. Throughout the rest of this paper we will be concerned with the second case—that in which the energy E_0 lies within the band and corresponds to a virtual level.

Friedel's analysis has convincingly demonstrated that such levels actually occur in alloy systems. Moreover, within the framework of our simple model it is quite easy to construct density-of-states functions that, for the correct choice of V_{mm} , lead to virtual levels for which $F_m'(E_0) < 0$. One such is derived from the band structure,

$$E(k) = 2\mathcal{E}(1)[\cos(k_x a) + \cos(k_y a) + \cos(k_z a)], \quad (10)$$

considered by Koster and Slater. These authors calculate the function $F_m(E)$ (which they call I_s) for this energy-vs-momentum relation. Their values indicate that the extrema of F_m lie within the band—thus, for appropriate values of V_{mm} , it gives rise to a virtual level of the type we desire. It is a simple matter to construct other examples. These do not, however, appear to be of great interest in their own right and we will not discuss them further, but merely assume the existence of a virtual level with $F_m'(E_0) < 0$. Our aim will be to investigate when and how this level polarizes as one introduces (in a self-consistent way) a spin-dependent potential in addition to V_{mm} . We shall also say a few words about the root of Eq. (9) at which $F_m' > 0$ (point *B* of Fig. 1). Our subsequent analysis will show, however, that such a virtual level does not polarize and is not, therefore, of great interest in the present connection.

III

We now return to Eq. (8)—assuming that it has a resonance (E_0) within the band at which $F_m'(E_0) < 0$ —

and consider the effect of adding a spin-dependent potential to V_{mm} . Since all quantities in our equations refer to the m th band we will, henceforth, drop this subscript and write the two potentials, for spin-up and spin-down electrons, as $V + \delta V_\uparrow$ and $V + \delta V_\downarrow$. From Eq. (8) the amplitudes at the impurity of the corresponding wave functions are (again dropping the subscript m)

$$U_\uparrow(\mathbf{R}_0) = e^{i\mathbf{k} \cdot \mathbf{R}_0} / \{ [1 - (V + \delta V_\uparrow)F(E)] - i\pi(V + \delta V_\uparrow)\rho(E) \}$$

and

$$U_\downarrow(\mathbf{R}_0) = e^{i\mathbf{k} \cdot \mathbf{R}_0} / \{ [1 - (V + \delta V_\downarrow)F(E)] - i\pi(V + \delta V_\downarrow)\rho(E) \}. \quad (11)$$

These wave functions are now used to calculate the change in the Hartree-Fock field of the impurity. Denoting this potential by V_{HF} , we have

$$\begin{aligned} V_{\text{HF}}a_\sigma(\mathbf{r} - \mathbf{R}_0) &= \sum_{\substack{\mathbf{k}'\sigma' \\ \text{(filled states)}}} \left\{ \int \psi_{\mathbf{k}'\sigma'}^*(\mathbf{r}') \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} \psi_{\mathbf{k}'\sigma'}(\mathbf{r}') a_\sigma(\mathbf{r} - \mathbf{R}_0) d^3r' \right. \\ &\quad \left. - \delta_{\sigma\sigma'} \int \psi_{\mathbf{k}'\sigma'}^*(\mathbf{r}') \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} \psi_{\mathbf{k}'\sigma'}(\mathbf{r}') a_\sigma(\mathbf{r}' - \mathbf{R}_0) d^3r' \right\}, \quad (12) \end{aligned}$$

and the matrix element $(a_\sigma(\mathbf{r} - \mathbf{R}_0), V_{\text{HF}}a_\sigma(\mathbf{r} - \mathbf{R}_0))$ is given by the expression

$$\begin{aligned} \sum_{\substack{\mathbf{k}'\sigma' \\ \text{(filled states)}}} &\left\{ \int \int a_\sigma^*(\mathbf{r} - \mathbf{R}_0) \psi_{\mathbf{k}'\sigma'}^*(\mathbf{r}') \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} \psi_{\mathbf{k}'\sigma'}(\mathbf{r}') \right. \\ &\quad \times a_\sigma(\mathbf{r} - \mathbf{R}_0) d^3r' d^3r - \delta_{\sigma\sigma'} \int \int a_\sigma^*(\mathbf{r} - \mathbf{R}_0) \\ &\quad \times \psi_{\mathbf{k}'\sigma'}^*(\mathbf{r}') \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} \psi_{\mathbf{k}'\sigma'}(\mathbf{r}') a_\sigma(\mathbf{r}' - \mathbf{R}_0) d^3r' d^3r \left. \right\}. \quad (13) \end{aligned}$$

To evaluate the integrals in this formula we use the expansion of $\psi_{\mathbf{k}'}$ given in Eq. (3). When this is substituted into Eq. (13) the biggest integrals come from terms in $\psi_{\mathbf{k}'}$ and $\psi_{\mathbf{k}'}^*$ that involve the Wannier function, $a(\mathbf{r} - \mathbf{R}_0)$, at the impurity atom. There will, of course, be matrix elements to other Wannier functions, but they are smaller and change relatively less when V goes to $V + \delta V$. This latter statement follows from Eq. (4) which indicates that, for $\mathbf{R}_i \neq \mathbf{R}_0$, $U(\mathbf{R}_i)$ is the sum of a plane wave of unit amplitude, and a scattered wave that changes as V goes to $V + \delta V$, but whose amplitude decreases with the distance, $|\mathbf{R}_i - \mathbf{R}_0|$. Since it is the change in V_{HF} that we wish to compute, we will ignore all contributions to Eq. (13) except those involving the Wannier function $a(\mathbf{r} - \mathbf{R}_0)$. With this approximation the direct and exchange integrals in Eq. (13) are the same and of the form

$$J = \int \int |a(\mathbf{r}-\mathbf{R}_0)|^2 |a(\mathbf{r}'-\mathbf{R}_0)|^2 \frac{e^2}{|\mathbf{r}-\mathbf{r}'|} d^3r d^3r'. \quad (14)$$

Thus, the parallel-spin Coulomb integral is cancelled by the exchange integral and Eq. (13) takes the form

$$(a_\uparrow(\mathbf{r}-\mathbf{R}_0), V_{\text{HF}} a_\uparrow(\mathbf{r}-\mathbf{R}_0)) = J \sum_{\mathbf{k}' \text{ (filled states)}} [|U_\downarrow(\mathbf{R}_0)|^2], \quad (15)$$

and

$$\delta V_\uparrow = J \sum_{\text{(filled states)}} \left\{ \frac{1}{[1-(V+\delta V_\downarrow)F(E)]^2 + \pi^2(V+\delta V_\downarrow)^2 \rho^2(E)} - \frac{1}{[1-VF(E)]^2 + \pi^2 V^2 \rho^2(E)} \right\}, \quad (16)$$

$$\delta V_\downarrow = J \sum_{\text{(filled states)}} \left\{ \frac{1}{[1-(V+\delta V_\uparrow)F(E)]^2 + \pi^2(V+\delta V_\uparrow)^2 \rho^2(E)} - \frac{1}{[1-VF(E)]^2 + \pi^2 V^2 \rho^2(E)} \right\}. \quad (17)$$

From these equations one sees that, as in Anderson's work, it is the Coulomb integral between antiparallel electrons that gives rise to polarization. It is clear from Eq. (13), however, that this interaction is spin dependent only because the Coulomb interaction between parallel-spin electrons is cancelled by the corresponding exchange interaction. Thus, in this rather backhanded

way, the polarization (if it exists) arises from the exchange interaction.

Our final task is to evaluate Eqs. (16) and (17), and relate the exchange potential to the properties of the virtual level that we have postulated. As in Eq. (6), the integrals involved in Eqs. (16) and (17) may be re-written as

$$\delta V_\uparrow = J \int_{-\infty}^{E_F} dE \rho(E) \left\{ \frac{1}{[1-(V+\delta V_\downarrow)F(E)]^2 + \pi^2(V+\delta V_\downarrow)^2 \rho^2(E)} - \frac{1}{[1-VF(E)]^2 + \pi^2 V^2 \rho^2(E)} \right\}, \quad (18)$$

$$\delta V_\downarrow = J \int_{-\infty}^{E_F} dE \rho(E) \left\{ \frac{1}{[1-(V+\delta V_\uparrow)F(E)]^2 + \pi^2(V+\delta V_\uparrow)^2 \rho^2(E)} - \frac{1}{[1-VF(E)]^2 + \pi^2 V^2 \rho^2(E)} \right\}, \quad (19)$$

where E_F is the Fermi level. The existence of a virtual level implies that $[1-VF(E)]=0$ for some value, $E=E_0$, within the band. If δV is not too large, and the level moderately sharp—and we will see that this must be so if there is to be any spin polarization—we may evaluate Eqs. (18) and (19) by expanding $F(E)$ about the point $E=E_0$ and setting $\rho(E) \simeq \rho(E_0) = \rho_0$. Thus we write

$$F(E) \simeq 1/V + (E-E_0)F'. \quad (20)$$

It is now a straightforward matter to calculate the integrals in Eqs. (18) and (19). One finds

$$\begin{aligned} \delta V_\uparrow = & \frac{J}{\pi(V+\delta V_\downarrow)^2 F'} \\ & \times \left\{ \tan^{-1} \left[\frac{F'(E_F-E_0)}{\pi \rho_0} + \frac{\delta V_\downarrow}{\pi \rho_0 V(V+\delta V_\downarrow)} \right] + \frac{\pi}{2} \right\} \\ & - \frac{J}{\pi V^2 F'} \left\{ \tan^{-1} \left[\frac{F'(E_F-E_0)}{\pi \rho_0} \right] + \frac{\pi}{2} \right\}, \quad (21) \end{aligned}$$

and a corresponding formula, with δV_\uparrow and δV_\downarrow interchanged, obtained by integrating Eq. (19).

We now examine these formulas in the limit where

$(\delta V/V)$ is small. This analysis will enable us to investigate the region in which the localized moment first appears or has small values (compared to one Bohr magneton). It is only in this range that our very simple model can be expected to have any validity. For larger moments, the potentials δV_\uparrow and δV_\downarrow are also large and the virtual level is shifted by many volts. Under these circumstances neither the one-band model, nor our simple assumption concerning the density of states [Eq. (20)], are even qualitatively correct.

With the assumption $\delta V/V \ll 1$, Eq. (21) takes the form

$$\delta V_\uparrow = (J/\pi V^2 F') \{ \tan^{-1}[(E_F-E_0)/\Delta + \delta V_\downarrow/\pi \rho_0 V^2] - \tan^{-1}[E_F-E_0/\Delta] \}, \quad (22)$$

where $\Delta = \pi \rho_0 / F'$ is the width of the virtual level. As before, there is also a corresponding equation with δV_\uparrow and δV_\downarrow interchanged. The meaning of these equations is best revealed by making plots of δV_\uparrow vs δV_\downarrow . We consider first the simplest case in which the virtual level lies at the Fermi level ($E_F=E_0$). The simultaneous equations then take the form

$$\begin{aligned} \delta V_\uparrow &= (J/\pi V^2 F') \tan^{-1}[\delta V_\downarrow/\pi \rho_0 V^2], \\ \delta V_\downarrow &= (J/\pi V^2 F') \tan^{-1}[\delta V_\uparrow/\pi \rho_0 V^2]. \end{aligned} \quad (23)$$

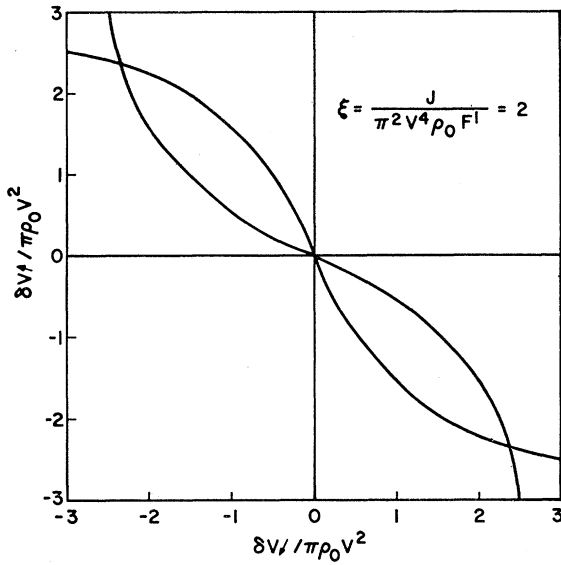


FIG. 2. δV_{\uparrow} vs δV_{\downarrow} for a case in which the virtual level is at the Fermi level, and polarized.

Typical plots of these equations (remembering that we have assumed $F' < 0$) are illustrated in Figs. 2 and 3. In the first case (Fig. 2) we have chosen $(J/\pi^2\rho_0 V^4 F') > 1$ and there are three sets of roots: an unstable one with $\delta V_{\uparrow} = \delta V_{\downarrow} = 0$, and two stable ones (corresponding to up or down spin of the localized moment) with $\delta V_{\uparrow} = -\delta V_{\downarrow} = \pm(\text{constant})$. On the other hand, in Fig. 3 we have assumed $|J/\pi^2\rho_0 V^4 F'| < 1$ and there is a single stable set of roots with $\delta V_{\uparrow} = \delta V_{\downarrow} = 0$, and no localized moment. Graphs for the case $E_F \neq E_0$ may be obtained from those with $E_F = E_0$ merely by sliding the two curves of δV_{\uparrow} vs δV_{\downarrow} the appropriate distance along the δV_{\uparrow} and

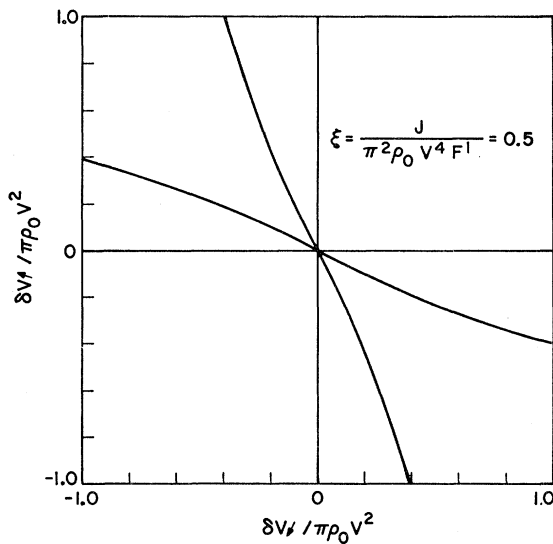


FIG. 3. δV_{\uparrow} vs δV_{\downarrow} for a case in which the virtual level is at the Fermi level, but unpolarized.

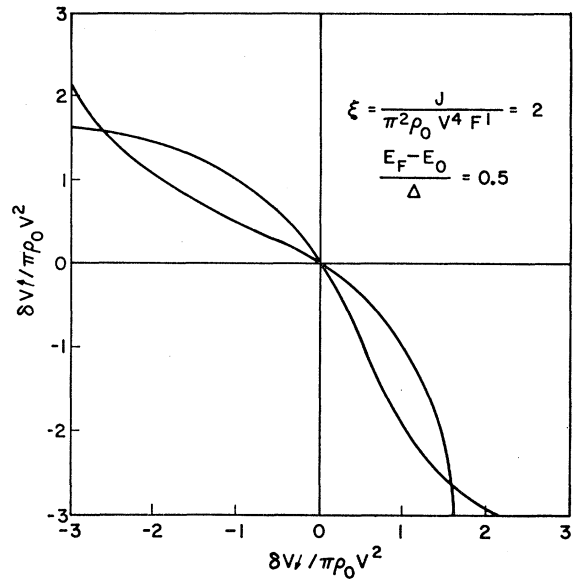


FIG. 4. δV_{\uparrow} vs δV_{\downarrow} for a case in which the virtual level is slightly displaced from the Fermi level, but remains polarized.

δV_{\downarrow} axes. For example, in Figs. 4 and 5 we illustrate two cases obtained from Fig. 2. In the former—in which the shift $(E_F - E_0)$ is fairly small—there remain three sets of roots, but now with the stable ones having $\delta V_{\uparrow} \neq -\delta V_{\downarrow}$. Figure 5 illustrates a case in which $(E_F - E_0)$ is larger, and there is no longer a localized moment. It is clear from these examples that the criterion for the existence of a moment is that $\partial(\delta V_{\uparrow})/\partial(\delta V_{\downarrow})$, as calculated from Eq. (22), be greater than unity. This condition is fulfilled if the inequality,

$$\frac{\Delta^2 + (E_F - E_0)^2}{\Delta^2} < \left| \frac{J}{\pi^2 V^4 \rho_0 F'} \right|, \quad (24)$$

is satisfied. It is interesting to make estimates of the quantity $|J/\pi^2 V^4 \rho_0 F'| = \xi$ for the band structure studied by Koster and Slater, using values of V that give rise to a virtual level. A virtual level with $F' < 0$ occurs when V is about one-third the bandwidth (E_B) . One then finds that ξ is about $(2J/E_B)$. Thus, with the right value of V and a fairly narrow band, it might be possible to obtain a localized moment in the band structure studied by Koster and Slater. This is not, in fact, a particularly favorable example for the occurrence of localized moments. These numerical estimates suggest, however, that it is possible to obtain localized moments with quite reasonable values of the parameters that appear in Eq. (24).

It remains to say a few words about the situation in which there is a virtual level near the Fermi level with $F'(E_0) > 0$. As in the previous case, one determines δV_{\uparrow} and δV_{\downarrow} by plotting these quantities against one another. Again, for $J/\pi^2 V^4 \rho_0 F' > \Delta^2 + (E_F - E_0)^2/\Delta^2$, there are three sets of roots but now, for each set, we find

$\delta V_{\uparrow} = \delta V_{\downarrow}$. Thus the equations tell us that our original Hartree-Fock potential was an unstable one and that V will so adjust itself as to reduce $J/\pi^2 V^4 \rho_0 F'$ below $\Delta^2 + (E_F - E_0)^2/\Delta^2$. The origin of this instability is clear from Fig. 2. If, for the root with $F' > 0$, one makes the potential more attractive (V more negative) the virtual level at B moves to *higher* energy. Thus, if the Fermi level lies near B , the electron density in the vicinity of the impurity is decreased by making V more attractive—which, in turn, makes V more attractive still.

IV. DISCUSSION

Equations (22)–(24), as well as Figs. 2–5, are entirely analogous in structure to those derived—and analyzed in considerable detail—by Anderson. In particular, one sees from Eq. (24) that, as in his work, the essential condition for a localized moment is the existence of a relatively sharp virtual level lying close to the Fermi level. As viewed from this point of view, the two theories appear equivalent. It is clear, however, that their origins are rather different. Anderson starts with a d state in a sea of mobile electrons and must, to preserve the individuality of the former, assume that its wave function is of a different character from those of the conduction electrons. We, on the other hand, adopt a one-band model which is equivalent to assuming that the wave function on the impurity is similar to those of the conduction electrons. In this sense the two approaches are complementary to one another—one might expect Anderson's to be more correct at the beginning of the $4d$ series, where the Fe atoms have a quite different number of d electrons from those of the matrix, whereas that described above might be more nearly applicable near its end.

Finally, we should say a word about the most basic property of a virtual level—the fact that it corresponds to a maximum in the scattering cross section. As Friedel has emphasized, if the virtual level occurs at the Fermi level it should give rise to an unusually large residual resistance. This, according to Anderson's and our models, is just the situation in those alloys in which the Fe

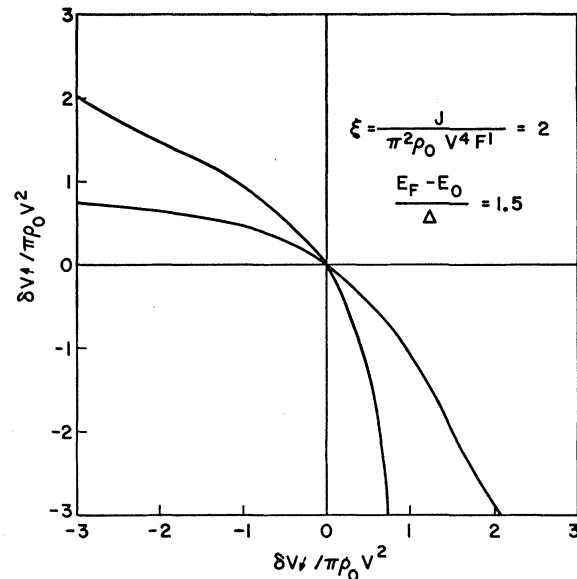


FIG. 5. δV_{\uparrow} vs δV_{\downarrow} for a case in which the virtual level is shifted far enough from the Fermi level to destroy polarization.

atoms first begin to acquire a moment. Thus, it would be exceedingly interesting to measure the residual resistance, due to Fe atoms, of the $4d$ elements and alloys studied in reference 1. This quantity should show a maximum for those alloys in which moments are just beginning to appear, but decrease as one goes to alloys with larger moments since, in them, the virtual level is split by the exchange potential and forced away from the vicinity of the Fermi surface. Such behavior would be similar to that of the $3d$ elements when dissolved in Cu, which has been extensively discussed by Friedel.

ACKNOWLEDGMENTS

The author would like to express his appreciation to P. W. Anderson, A. M. Clogston, and B. T. Matthias for a number of stimulating conversations on the topics discussed in this paper.