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Ferromagnetism of Transition-Metal Alloys*

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By extending Anderson's model for a single impurity in a metal to the case of a finite concentration of impurities, the electronic structure and the electron interaction in transition-metal alloys are studied. The local-environment effect in the impurity magnetization first discussed by Jaccarino and Walker can be reasonably explained by accounting for the local modification of the electronic structure of the host metal due to the other surrounding impurities. In alloys such as Ni in Pd, where in the low-concentration limit the Ni impurity does not have a localized moment and the alloy system is not ferromagnetic, we examine how, as we increase the impurity concentration, the total ferromagnetism of the alloy is produced. If the interactions among the impurities, between the impurities and the host metal, and among the host-metal electrons are properly taken into account, the Friedel-Anderson-Wolff condition for the occurrence of the localized magnetic moment on an impurity exactly coincides with the condition for the onset of ferromagnetism of the entire system. Various magnetic properties of transition-metal alloys are discussed, taking into account the simultaneous modifications of electronic structure and electron interaction due to the presence of impurities.

I. INTRODUCTION

In spite of extensive efforts, we still do not have a satisfactory understanding of some of the basic properties of transition-metal alloys. The alloys $Pd_{1-x}Ni_x$,[1-7] $Rh_{1-x}Ni_x$,[8-10] and $Cu_{1-x}Ni_x$,[11-13] for instance, have a common interesting feature, namely, when the concentration of Ni is lower than a certain critical value x_{crit}, the alloys are not ferromagnetic at any temperature, and, for $x>x_{\text{crit}}$, they become ferromagnetic at low temperatures. It is supposed that, for $x<x_{\text{crit}}$, Ni does not have a localized moment. The concept of a critical concentration raises many questions: Is the localized moment formed on Ni for $x>x_{\text{crit}}$ even above the Curie temperature? What is the mechanism of ferromagnetism? Which electrons are the carrier of ferromagnetism for $x>x_{\text{crit}}$, those associated with the impurities, the host-metal electrons, or both? How is the formation of a localized moment on the Ni related to the over-all ferromagnetism?

Some more detailed experimental analysis has been made on other systems. From the Pd concentration dependence of the Co^{59} NMR in the $Rh_{1-x}Pd_x$ host, Jaccarino and Walker[14] suggested that the magnetization of a Co impurity takes place discontinuously when a Co impurity happens to have two or more Pd atoms in the nearest-neighbor sites. Many alloy systems have been found in which the magnetic behavior of an atom seems to depend sensitively on the immediate local environment as well as the bulk properties of the host metals. Those alloy systems include Fe or Co in NbMo,[15,15a] Fe or Co in Al,[16-18] Ni in Cu,[12,13] and V in Au.[19-22]

The purpose of this paper is to understand problems such as those mentioned in the above two paragraphs. Let us consider the $Pd_{1-x}Ni_x$ system, for example. When the Ni concentration is below ~2 at.%, we observe neither a "localized moment" on the Ni atom nor ferromagnetism of the system. To explain this behavior, we must first understand the problem of a single impurity in a metal by determining what happens to the Ni impurity atom and the host-metal Pd. This single-impurity problem was first formulated by Friedel[23] and further

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developed by Anderson,[24] Wolff,[25] and others.[26] In this paper, we adopt the Anderson-model approach. In terms of the Anderson model, the atomic level of Ni impurity is broadened through the interaction with the conduction electrons ($4d$,$5s$) of the Pd metal to such an extent that the Ni impurity can no longer maintain a localized magnetic moment. The original theory of Friedel, Anderson, and Wolff stops just at this stage of the single-impurity problem, and thus, we cannot answer what happens if we increase the Ni concentrations gradually. Some of the many-impurity effects in the Anderson model have already been discussed,[27–31] but these papers assumed localized moments were present and considered the effective exchange interaction between the localized magnetic moments through an indirect mechanism via the conduction electrons[27,28] or a direct transfer between neighboring impurities.[29–31] The purpose of this paper is different. Namely, we wish to understand why whether an impurity has a localized moment or not depends on the impurity concentration or, more generally, on the immediate atomic environment around the impurity, and what is the relation between the formation of localized moment and the ferromagnetism of the alloy system.

Generally speaking, a metal is characterized by two kinds of quantities: the electronic structure and the electron interaction. To obtain the spin susceptibility of a metal, we have to know both the density of states at the Fermi surface (electronic structure) and the effective exchange interaction (electron interaction). The situation is the same in a description of the behavior of alloys and there have been papers which consider either aspect of the problem. For instance, electron interaction in alloys was discussed based on various models.[32–34] Recently, the modification of host-metal bands due to the presence of impurity potentials was also discussed.[35] In this paper, both aspects of the problem, the electronic structure and the electron interaction, are treated on the same footing starting from Anderson's model.

In Sec. II, we extend Anderson's original model to the many-impurity case. Since for many of the alloy systems being considered the host metals also are transition metals where the Coulomb interaction is very important, we also include the Coulomb interaction between host-metal electrons. With these two extensions of Anderson's model, in Sec. III, the Green's functions of the impurity and host metal electrons are calculated with the Hartree-Fock approximation.

Using the result of Sec. III, one possible mechanism of the local-environment effects for the magnetization of an impurity is discussed in Sec. IV. The distortion of the host-metal density of states due to the presence of impurities is different for different impurity sites, since each impurity has a different local environment. Note that the width of an impurity state is determined by the density of states of the host metal at the site of the impurity. This fact can explain the local-environment effect. In obtaining this conclusion, we noticed that, in some cases, even for a nearest-neighbor pair of impurities, the indirect interaction via a host-metal conduction electron can dominate the direct-transfer interaction. Another possible mechanism of the local environment effect which comes from the effective exchange interaction between impurities is discussed in Sec. V.

In Sec. V, we start by assuming that in the single-impurity limit the impurity does not have a localized moment and the entire alloy is not ferromagnetic at any temperature, i.e., Ni in Pd. We study how the onset of the total ferromagnetism of the alloy and the occurrence of a localized moment on the impurity are produced as we increase the impurity concentration. The criterion for the formation of a localized moment is the divergence of the impurity susceptibility (the Friedel-Anderson-Wolff criterion[23–25]). The condition for the ferromagnetism of the alloy is the divergence of the total susceptibility. In calculating the magnetic susceptibilities of the localized states and the host metal by the Hartree-Fock approximation, we find they are coupled to each other. From the coupled equation for the susceptibilities, we find that all three susceptibilities, that of the individual impurities, the system of all the impurities and the host-metal electrons, diverge together at the critical impurity concentration (or at the Curie temperature). In a sense, the ferromagnetism (or antiferromagnetism) of the entire alloy and the formation of a localized moment on the impurity occur at the same impurity concentration (or temperature). The above observation, especially concerning the formation of a localized moment on an impurity, should always be understood in the sense of the Friedel-Anderson-Wolff criterion. As will be seen later, however, the Friedel-Anderson-Wolff criterion may not be the appropriate one in the case of many impurities.

In Sec. VI, we analyze some of the experimental data on alloys like PdNi, PdRh, and RhNi based on the results of Sec. V. In the presence of this analysis, we show that it is really important to consider both the electronic structure and the electron interaction properly. For instance, the denominator for the alloy sus-

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ceptibility (which is the inverse of the exchange-enhancement factor) contains terms quadratic in the impurity concentration. One power comes from the electron interaction and the other from the change of the electronic structure (density of states). This quadratic dependence in impurity concentration seems to be essential in order to understand the experimental situation.

II. MODEL

In this paper, we use Anderson's model generalized in the following two points: (1) We consider many mutually interacting (N_0) impurities instead of a single one. More generally, these impurities need not be of the same species. Namely, we consider the case that there are two or more different kinds of impurities. (2) We include the Coulomb interaction between the conduction electrons of the host metal since as the host-metal we are interested in such metal as Pd where the Coulomb interaction is very important. With these two modifications, the Hamiltonian is

$$\mathcal{H}=\mathcal{H}_k+\mathcal{H}_c+\mathcal{H}_d+\mathcal{H}_{dd}+\mathcal{H}_{cd}+\mathcal{H}_t\,, \tag{2.1}$$

where $\mathcal{H}_k$ and $\mathcal{H}_c$ are, respectively, the one-particle energy and the Coulomb repulsion-energy of the host-metal conduction electrons:

$$\mathcal{H}_k=\sum_{k\sigma} \epsilon_k c_{k\sigma}{}^\dagger c_{k\sigma}\,, \tag{2.2}$$

$$\mathcal{H}_c=\tfrac{1}{2}v \sum_{\substack{k,k'\\ \sigma,\sigma'}}{}' c_{k\sigma}{}^\dagger c_{k'\sigma'}{}^\dagger c_{k'-q,\sigma'}c_{k+q,\sigma}\,. \tag{2.3}$$

Here the host-metal conduction band is represented by a nondegenerate band, although, in a transition-metal host, we actually refer to the orbitary degenerate $3d$ or $4d$ electrons as conduction electrons. $c_{k\sigma}{}^\dagger$ is the creation of the conduction electron with energy ϵ_k and spin $\sigma(=+ \text{ or } -)$. The Coulomb interaction is simplified by using a δ-function interaction. The prime on the summation in Eq. (2.3) means to exclude $q=0$ from the summation. $\mathcal{H}_d$ and $\mathcal{H}_{dd}$ are, respectively, the one-particle energy and the Coulomb repulsion of electrons at the impurity:

$$\mathcal{H}_d=\sum_{i,\sigma} E_i{}^0 d_{i\sigma}{}^\dagger d_{i\sigma}\,, \tag{2.4}$$

$$\mathcal{H}_{dd}=\sum_{i} U_i d_{i+}{}^\dagger d_{i+}d_{i-}{}^\dagger d_{i-}\,, \tag{2.5}$$

where again we approximate the ith impurity level by a nondegenerate single-energy level $E_i{}^0$ and the $d_{i\sigma}{}^\dagger$ is the creation operator of a σ spin electron at the ith impurity. Here the suffix i on $E_i{}^0$ means that $E_i{}^0$ depends on the species of the ith impurity. $E_i{}^0$'s of the same kind of impurities are equal. U_i is the Coulomb repulsion between electrons of opposite spins at the ith impurity site and it also can depend on the species of the impurity. $\mathcal{H}_{cd}$ is the interaction term between the conduction electron and the impurity electron (s-d mixing):

$$\mathcal{H}_{cd}=\sum_{i,k,\sigma} (V_{ik}d_{i\sigma}{}^\dagger c_{k\sigma}+V_{ik}{}^* c_{k\sigma}{}^\dagger d_{i\sigma})\,, \tag{2.6}$$

$$V_{ik}=V_i(k)\exp(ikR_i)\,, \tag{2.7}$$

where R_i is the ith impurity site. $V_i(k)$ is defined by Anderson[24] and it is k-dependent. In our calculation, as in the case of many other authors, we will neglect the k dependence of $V_i(k)$ and put $V_i(k)=V_i$, and for simplicity we assume it to be real.

The last term in the Hamiltonian is the direct-transfer integral between the impurities[29]:

$$\mathcal{H}_t=\sum_{i,j,\sigma} T_{ij}d_{i\sigma}{}^\dagger d_{j\sigma}\,. \tag{2.8}$$

In general, T_{ij} depends on the species of the ith and the jth impurities as well as the distance between them. Notice that T_{ij} is real and $T_{ii}=0$.

III. CALCULATIONS OF GREEN'S FUNCTIONS

In order to calculate the physical properties of localized and conduction electrons, we introduce the two-time retarded Green's function of two Fermion operators a and $b^\dagger$,[36] whose Fourier transform is denoted as $\langle a|b^\dagger\rangle_\omega$. The prescription to calculate the thermodynamical average $\langle b^\dagger a\rangle$ from the corresponding Green's function is given by

$$\langle b^\dagger a\rangle=-\frac{1}{2\pi i}\int_{-\infty}^{\infty} d\omega\{\langle a|b^\dagger\rangle_{\omega+i0^+} -\langle a|b^\dagger\rangle_{\omega-i0^+}\}f(\omega)\,, \tag{3.1}$$

where $f(\omega)$ is the Fermi distribution function of the system. The Green's function is obtained by solving its equation of motion

$$\omega\langle a|b^\dagger\rangle_\omega=\langle[a,b^\dagger]_+\rangle+\langle[a,\mathcal{H}]|b^\dagger\rangle_\omega\,, \tag{3.2}$$

where $[\,,\,]_+$ and $[\,,\,]$ are the anticommutator and commutator and ω is always understood to be $\omega+i0^+$. In the last term on the right-hand side of Eq. (3.2), $\mathcal{H}$ should be replaced by $\mathcal{H}-\mu\mathfrak{N}$, where μ is the chemical potential and $\mathfrak{N}$ is the operator of the total number of electrons in the system. We can eliminate $\mu\mathfrak{N}$ by measuring every energy level form the chemical potential.

The necessary Green's functions to be calculated are of the type $\langle d_{i\sigma}|d_{j\sigma}{}^\dagger\rangle_\omega$ and $\langle c_{k\sigma}|c_{k'\sigma}{}^\dagger\rangle_\omega$. In the procedure of calculating them, however, Green's functions of following type also appear: $\langle d_{i\sigma}|c_{k'\sigma}{}^\dagger\rangle_\omega$ and $\langle c_{k\sigma}|d_{j\sigma}{}^\dagger\rangle_\omega$. We set up the equations of motion for all these Green's functions. The calculation is similar to that we presented previously[27] except for the modifications mentioned in the previous sections: (1) the inclusion of the Coulomb interaction between the conduction electrons of the host metal, (2) the presence of

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more than two different kinds of impurities, (3) the inclusion of the direct transfer term between impurities, and (4) the presence of an external magnetic field. The effect of an external field is incorporated simply by modifying ϵ_k and E_i^0 to

$$\epsilon_{k\pm}=\epsilon_k\pm\mu_B H\,,\quad E_{i\pm}{}^0=E_i^0\pm\mu_B H\,, \tag{3.3}$$

where H is the external magnetic field applied in the z direction and μ_B is the Bohr magneton (>0). We assume the g factors of the impurity and host-metal electrons are the same and equal to 2. The set of the equations of motions are

$$\begin{aligned}(\omega-E_{i+}{}^0)\langle d_{i+}|d_{j+}{}^\dagger\rangle_\omega
&=\delta_{ij}+V_i\sum_k e^{ikR_i}\langle c_{k+}|c_{j+}{}^\dagger\rangle_\omega+\sum_{j'}T_{ij'}\langle d_{j'+}|d_{j+}{}^\dagger\rangle_\omega\\
&\qquad+\langle[d_{i+},\mathcal{H}_{dd}]|d_{j+}{}^\dagger\rangle_\omega\,,\end{aligned} \tag{3.4}$$

$$(\omega-\epsilon_{k+})\langle c_{k+}|d_{j+}{}^\dagger\rangle_\omega=\sum_i V_i e^{-ikR_i}\langle d_{i+}|d_{j+}{}^\dagger\rangle_\omega+\langle[c_{k+},\mathcal{H}_c]|d_{j+}{}^\dagger\rangle_\omega\,, \tag{3.5}$$

$$(\omega-\epsilon_{k+})\langle c_{k+}|c_{k'+}{}^\dagger\rangle_\omega=\delta_{k,k'}+\sum_i V_i e^{-ikR_i}\langle d_{i+}|c_{k'+}{}^\dagger\rangle_\omega+\langle[c_{k+},\mathcal{H}_c]|c_{k'+}{}^\dagger\rangle_\omega\,, \tag{3.6}$$

$$\begin{aligned}(\omega-E_i^0)\langle d_{i+}|c_{k'+}{}^\dagger\rangle_\omega
&=V_i\sum_k e^{ikR_i}\langle c_{k+}|c_{k'+}{}^\dagger\rangle_\omega+\sum_j T_{ij}\langle d_{j+}|c_{k'+}{}^\dagger\rangle_\omega\\
&\qquad+\langle[d_{i+},\mathcal{H}_{dd}]|c_{k'}{}^\dagger{}_+\rangle_\omega\,.\end{aligned} \tag{3.7}$$

The equations for a spin-down electron Green's function are obtained simply by changing spin indices from ± to ∓ in the above set of equations.

In order to solve the above set of equations, we introduce the Hartree-Fock approximation to the following four Green's functions appearing in the above set of equations: $\langle[d_{i+},\mathcal{H}_{dd}]|d_{j+}{}^\dagger\rangle_\omega$, $\langle[c_{k+},\mathcal{H}_c]|d_{j+}{}^\dagger\rangle_\omega$, $\langle[c_{k+},\mathcal{H}_c]|c_{k'+}{}^\dagger\rangle_\omega$, and $\langle[d_{i+},\mathcal{H}_{dd}]|c_{k'+}{}^\dagger\rangle_\omega$. First, we notice the commutator

$$[d_{i+},\mathcal{H}_{dd}]=U_i d_{i+}d_{i-}{}^\dagger d_{i-}\,, \tag{3.8}$$

$$[c_{k+},\mathcal{H}_c]=v\sum_{l,q,\sigma}{}' c_{l\sigma}{}^\dagger c_{l+q,\sigma}c_{k-q,+}\,, \tag{3.9}$$

where the prime on the summation in Eq. (3.9) indicates to exclude $q=0$. The Hartree-Fock approximation for $\langle[d_{i+},\mathcal{H}_{dd}]|d_{j+}{}^\dagger\rangle_\omega$ is as follows:

$$\begin{aligned}\langle[d_{i+},\mathcal{H}_{dd}]|d_{j+}{}^\dagger\rangle_\omega
&=U_i\langle d_{i+}d_{i-}{}^\dagger d_{i-}|d_{j+}{}^\dagger\rangle_\omega\\
&\cong U_i\langle d_{i-}{}^\dagger d_{i-}\rangle\langle d_{i+}|d_{j+}{}^\dagger\rangle_\omega-U_i\langle d_{i-}{}^\dagger d_{i+}\rangle\langle d_{i-}|d_{j+}{}^\dagger\rangle_\omega\\
&\cong U_i N_{i-}\langle d_{i+}|d_{j+}{}^\dagger\rangle_\omega\,,\end{aligned} \tag{3.10}$$

where $N_{i\pm}\equiv\langle d_{i\pm}{}^\dagger d_{i\pm}\rangle$ is to be determined self-consistently. Similarly,

$$\begin{aligned}\langle[d_{i+},\mathcal{H}_{dd}]|c_{k'+}{}^\dagger\rangle_\omega
&=U_i\langle d_{i+}d_{i-}{}^\dagger d_{i-}|c_{k'+}{}^\dagger\rangle_\omega\\
&\cong U_i\langle d_{i-}{}^\dagger d_{i-}\rangle\langle d_{i+}|c_{k'+}{}^\dagger\rangle_\omega-\langle d_{i-}{}^\dagger d_{i+}\rangle\langle d_{i-}|c_{k'+}{}^\dagger\rangle_\omega\\
&\cong U_i N_{i-}\langle d_{i+}|c_{k'+}{}^\dagger\rangle_\omega\,,\end{aligned} \tag{3.11}$$

$$\begin{aligned}\langle[c_{k+},\mathcal{H}_c]|c_{k'+}{}^\dagger\rangle_\omega
&=v\sum_{l,q,\sigma}{}'\ \langle c_{l\sigma}{}^\dagger c_{l+q,\sigma}c_{k-q,+}|c_{k'+}{}^\dagger\rangle_\omega\\
&\cong v\sum_{l,q,\sigma}{}'\ \langle c_{l\sigma}{}^\dagger c_{l+q,\sigma}\rangle\langle c_{k-q,+}|c_{k'+}{}^\dagger\rangle_\omega\\
&\qquad-v\sum_{l,q,\sigma}{}'\ \langle c_{l\sigma}{}^\dagger c_{k-q,+}\rangle\langle c_{l+q,\sigma}|c_{k'+}{}^\dagger\rangle_\omega\\
&\cong v\sum_l\langle c_{l-}{}^\dagger c_{l+k-k',-}\rangle\langle c_{k'+}|c_{k'+}{}^\dagger\rangle_\omega(1-\delta_{kk'})\\
&\qquad-v\sum_q{}'\langle c_{k-q,+}{}^\dagger c_{k-q,+}\rangle\langle c_{k+}|c_{k'+}{}^\dagger\rangle_\omega\,,\end{aligned} \tag{3.12}$$

$$\begin{aligned}\langle[c_{k+},\mathcal{H}_c]|d_{j+}{}^\dagger\rangle_\omega
&=v\sum_{l,q,\sigma}{}'\ \langle c_{l\sigma}{}^\dagger c_{l+q,\sigma}c_{k-q,+}|d_{j+}{}^\dagger\rangle_\omega\\
&\cong v\sum_{l,q,\sigma}{}'\ \langle c_{l\sigma}{}^\dagger c_{l+q,\sigma}\rangle\langle c_{k-q,+}|d_{j+}{}^\dagger\rangle_\omega\\
&\qquad-v\sum_{l,q,\sigma}{}'\ \langle c_{l\sigma}{}^\dagger c_{k-q,+}\rangle\langle c_{l+q,\sigma}|d_{j+}{}^\dagger\rangle_\omega\\
&\cong -v\sum_q{}'\ \langle c_{k-q,+}{}^\dagger c_{k-q,+}\rangle\langle c_{k+}|d_{j+}{}^\dagger\rangle_\omega\,.\end{aligned} \tag{3.13}$$

With these approximations, Eqs. (3.10)–(3.13), the set of equations of motion, Eqs. (3.4)–(3.7), is reduced to

$$\begin{aligned}(\omega-E_{i\pm}{}^0-U_iN_{i\mp})\langle d_{i\pm}|d_{j\pm}{}^\dagger\rangle_\omega
&=\delta_{ij}+V_i\sum_k e^{ikR_i}\langle c_{k\pm}|d_{j\pm}{}^\dagger\rangle_\omega\\
&\qquad+\sum_{j'}T_{ij'}\langle d_{j'\pm}|d_{j\pm}{}^\dagger\rangle_\omega\,,\end{aligned} \tag{3.4$'$}$$

$$(\omega-\epsilon_{k\pm}+vn_\pm)\langle c_{k\pm}|d_{j\pm}{}^\dagger\rangle_\omega=\sum_i V_i e^{-ikR_i}\langle d_{i\pm}|d_{j\pm}{}^\dagger\rangle_\omega\,, \tag{3.5$'$}$$

$$\begin{aligned}(\omega-\epsilon_{k\pm}+vn_\pm)\langle c_{k\pm}|c_{k'\pm}{}^\dagger\rangle_\omega
&=\delta_{kk'}+\sum_i V_i e^{-ikR_i}\langle d_{i\pm}|c_{k'\pm}{}^\dagger\rangle_\omega\\
&\qquad+vn_\mp(k-k')\langle c_{k'\pm}|c_{k'\pm}{}^\dagger\rangle_\omega(1-\delta_{kk'})\,,\end{aligned} \tag{3.6$'$}$$

$$\begin{aligned}(\omega-E_{i\pm}{}^0-U_iN_{i\mp})\langle d_{i\pm}|c_{k'\pm}{}^\dagger\rangle_\omega
&=V_i\sum_k e^{ikR_i}\langle c_{k\pm}|c_{k'\pm}{}^\dagger\rangle_\omega+\sum_j T_{ij}\langle d_{j\pm}|c_{k'\pm}{}^\dagger\rangle_\omega\,,\end{aligned} \tag{3.7$'$}$$

where $n_\pm=\sum_k\langle c_{k\pm}{}^\dagger c_{k\pm}\rangle$ and $n_\pm(q)=\sum_k\langle c_{k\pm}{}^\dagger c_{k+q,\pm}\rangle$, which must also be determined self-consistently. The coupled equations, Eqs. (3.4′)–(3.7′), are solved:

$$\langle d_{i\pm}|d_{i\pm}^{\dagger}\rangle_{\omega}=\Big(\omega-E_{i\pm}{}^{0}-U_iN_{i\mp}-V_i{}^2F_{0\pm}(\omega)-\sum_{j(\neq i)}[V_iV_jF_{ij\pm}(\omega)+T_{ij}]$$

$$\times\frac{1}{\omega-E_{j\pm}{}^{0}-U_jN_{j\mp}-V_j{}^2F_{0\pm}(\omega)}[V_jV_iF_{ji\pm}(\omega)+T_{ji}]\Big)^{-1},\quad(3.14)$$

$$\langle c_{k\pm}|c_{k'\pm}^{\dagger}\rangle_{\omega}=\frac{\delta_{kk'}}{\omega-\epsilon_{k\pm}+vn_{\pm}}+\frac{1}{\omega-\epsilon_{k\pm}+vn_{\pm}}\frac{1}{\omega-\epsilon_{k'\pm}+vn_{\pm}}\sum_i V_i{}^2e^{-i(k-k')R_i}\langle d_{i\pm}|d_{i\pm}^{\dagger}\rangle_{\omega}+vn_{\mp}(k-k')$$

$$\times\langle c_{k'\pm}|c_{k'\pm}^{\dagger}\rangle_{\omega}(1-\delta_{kk'})\frac{1}{\omega-\epsilon_{k\pm}+vn_{\pm}}+\sum_{i\neq j}V_iV_j\frac{e^{-ikR_i}}{\omega-\epsilon_{k\pm}+vn_{\pm}}\langle d_{i\pm}|d_{i\pm}^{\dagger}\rangle_{\omega}[V_iV_jF_{ij\pm}(\omega)+T_{ij}]$$

$$\times\frac{1}{\omega-E_{j\pm}{}^{0}-U_jN_{j\mp}-V_j{}^2F_{0\pm}(\omega)}\frac{e^{ik'R_j}}{\omega-\epsilon_{k'\pm}+vn_{\pm}},\quad(3.15)$$

where

$$F_{ij\pm}(\omega)=\sum_k\frac{e^{ikR_{ij}}}{\omega-\epsilon_{k\pm}+vn_{\pm}+i0^+},\quad R_{ij}=R_i-R_j,\quad(3.16)$$

$$F_{0\pm}(\omega)=\sum_k\frac{1}{\omega-\epsilon_{k\pm}+vn_{\pm}+i0^+}\equiv I_{c\pm}{}^{0}(\omega)-i\pi\rho_{c\pm}{}^{0}(\omega),$$

$$I_{c\pm}{}^{0}(\omega)=\sum_k P\frac{1}{\omega-\epsilon_{k\pm}+vn_{\pm}}.\quad(3.17)$$

In Eq. (3.17), $\rho_{c\pm}{}^{0}(\omega)$ is the density of states of the conduction electrons of the pure host metal and $I_{c\pm}{}^{0}(\omega)$ is the real part of $F_{0\pm}(\omega)$. Note that in the paramagnetic state when there is no external magnetic field we can drop the spin indices ± from the various quantities introduced in this section. Therefore, throughout this paper, we neglect the spin indices whenever we refer to quantities at zero external magnetic field.

If the Coulomb interaction v and the direct transfer between impurities T_{ij} are set equal to zero, and the difference in the species of impurities is neglected in Eqs. (3.14) and (3.15), one obtains the previous result of Ref. 27. In the following sections, we discuss various problems on the basis of our Green's functions, Eqs. (3.14) and (3.15).

IV. LOCAL-ENVIRONMENT EFFECTS

Since Jaccarino and Walker's interesting proposal, that the magnetization of an impurity takes place discontinuously depending on the atomic configuration in the immediate vicinity of the impurity, a number of systems similar to theirs have been discussed.[14–22] For instance, very recently in studying AuV alloys,[19–21] a number of people suggested that a V atom has a localized magnetic moment when it does not have V neighbors within a critical distance, say nearest-neighbor site, and the moment disappears if another V atom is on the nearest-neighbor site. Although this is a situation opposite to the case mentioned in the Introduction, the nature of the problem is exactly the same, namely, whether an impurity has a localized moment depends on the details in the immediate vicinity of the impurity. Some qualitative discussions[27,28,37] were made previously on this problem. We present a new simple explanation. Namely, based on Anderson's model, we consider how the width of the localized state of the ith impurity $\Delta_i{}^0$, which appears in the criterion for the formation of a local moment, is modified by the presence of the other surrounding impurities.

In the presence of other impurities, the density of states at the Fermi surface of the ith impurity is modified from $\rho_i{}^0(0)$ to $\rho_i(0)$. The situation that the single impurity does not have a local moment, but obtains a moment if the impurity has certain number of other impurities in its neighbors, can be described by the condition (see Sec. V)[24]: In case I,

$$U_i\rho_i{}^0(0)<1,\quad\text{but}\quad U_i\rho_i(0)\geqq 1.\quad(4.1)$$

Therefore, our problem is to discuss whether the situation described by Eq. (4.1) is likely to occur in the alloy system as studied by Jaccarino and others.[14–22] As will be shown, the change in the impurity density of states can be negative as well as positive. Thus, a situation opposite to Eq. (4.1) is also possible: In case II,

$$U_i\rho_i{}^0(0)\geqq 1,\quad\text{but}\quad U_i\rho_i(0)<1.\quad(4.2)$$

The case of V in Au may belong to case II. Note in Eqs. (4.1) and (4.2) that the impurity density of states is for the spin-unsplit states.

If the center of the impurity state is very near the Fermi level, Eqs. (4.1) and (4.2) can be rewritten in terms of the change in the width of the impurity states from $\Delta_i{}^0$ to $\Delta_i=\Delta_i{}^0+\delta\Delta_i$ [see Eq. (5.8)]. Corresponding to Eq. (4.1), for example, we have case I′:

$$U_i/\pi\Delta_i{}^0<1,\quad\text{but}\quad U_i/\pi(\Delta_i{}^0+\delta\Delta_i)\geq 1.\quad(4.1')$$

The physical origin of the change of the impurity state can be traced to the last term in the bracket on the right-hand side of Eq. (3.14), which represents the

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[37] M. Inoue and T. Moriya, Progr. Theoret. Phys. (Kyoto) **38**, 41 (1967).

interaction energy of the ith impurity with the surrounding other impurities and does not appear in the single-impurity limit

$$\Sigma_{i\pm}(\omega)=\sum_{j(\neq i)}\left[V_iV_jF_{ij\pm}(\omega)+T_{ij}\right]^2 \times\frac{1}{\omega-E_{j\pm}{}^0-U_jN_{j\mp}-V_j{}^2F_{0\pm}(\omega)}. \tag{4.3}$$

In Eq. (4.3), we used the fact that $F_{ij}(\omega)=F_{ji}(\omega)$ which is valid if $\epsilon_k=\epsilon_{-k}$, as is clear from the definition Eq. (3.16). The real and imaginary parts of Σ_i give the energy shift and change in the width of the impurity state. Our problem is to see how the impurity density of states is modified from $\rho_i{}^0$ to ρ_i by the effect of Σ_i.

Note that the approximation that the impurity density of states is a Lorentzian is a very crucial simplification. Although many important results have been obtained by using the fact that the impurity density of states is not a simple Lorentzian,[27–31] we use the Lorentzian approximation which makes the discussion for the change of an impurity state simple and transparent. Another technical justification for our procedure is that the ω dependence of $\Sigma_i(\omega)$ is not much sharper than the ω dependence of the single impurity term $V_i{}^2F_0(\omega)$, since in transition metals it is likely that the impurity-state width is not much smaller than the host-metal bandwidth. This can be discussed in two ways. First, as shown in the Appendix, we can carry out the summation over j in Eq. (4.3). Although $F_{ij}(\omega)$ is a rapidly oscillating function of ω for large R_{ij}, after the summation over j, the resultant ω dependence becomes essentially that of $F_0(\omega)$ or the impurity Green's function in the single-impurity limit [see Eq. (A4)]. Second, as follows in this section, we may retain only certain contributions in the summation over j, for instance, from nearest-neighbor impurities. The contribution from distant j's are small and likely to cancel each other. Within this approximation, the resulting ω dependence of $\Sigma_i(\omega)$ is again not sharp. Note, however, that we are not advocating neglecting the ω dependence in $\Sigma_i(\omega)$. What we have tried to illustrate is that the full inclusion of the ω dependence in $\Sigma_i(\omega)$ is about as important as the ω dependence of the single-impurity term $V_i{}^2F_0(\omega)$ and not much more.

Even within this approximation of a Lorentzian density of states, however, a fully self-consistent quantitative discussion for the general case is very difficult. If we change the width from $\Delta_i{}^0$ to $\Delta_i{}^0+\delta\Delta_i$ with fixed E_i (by E_i we imply the actual impurity energy level modified from $E_i{}^0$ by various effects), the number of electrons in the localized impurity state would change and this change complicates the problem. Since, for the moment, we are interested in the qualitative aspect of the problem, we assume that E_i is just as the chemical potential. In the following part of this section, the discussion will be focused exclusively on obtaining Eqs. (4.1′) and (4.2′) which would be clear from Eq. (4.2). Then our task is simply to estimate the change in the width of the ith impurity state which is the imaginary part of $\Sigma_i(\omega)$ (as to the effect of the real part of Σ_i we discuss in Sec. V).

As seen from Eq. (4.3), the change in the width consists of three different contributions corresponding to the three different components in the interaction energy $\Sigma_i(\omega)$:

$$\begin{aligned}\delta\Delta_i&=-\mathrm{Im}\Sigma_i(\omega)\\&=\delta\Delta_i{}^{(1)}+\delta\Delta_i{}^{(2)}+\delta\Delta_i{}^{(3)},\end{aligned} \tag{4.4}$$

$$\delta\Delta_i{}^{(1)}=-V_i{}^2\,\mathrm{Im}\left(\sum_{j(\neq i)}V_j{}^2\frac{1}{\omega-E_j{}^0-U_jN_j-V_j{}^2F_0(\omega)}F_{ij}(\omega)^2\right), \tag{4.5}$$

$$\delta\Delta_i{}^{(2)}=-\sum_{j(\neq i)}T_{ij}{}^2\,\mathrm{Im}\left(\frac{1}{\omega-E_j{}^0-U_jN_j-V_j{}^2F_0(\omega)}\right), \tag{4.6}$$

$$\delta\Delta_i{}^{(3)}=-2\sum_{j(\neq i)}V_iV_jT_{ij}\,\mathrm{Im}\left(F_{ij}(\omega)\frac{1}{\omega-E_j{}^0-U_jN_j-V_j{}^2F_0(\omega)}\right). \tag{4.7}$$

In the above equations, we put $H=0$ and, therefore, $N_{i+}=N_{i-}\equiv N_i$, etc. Note that the expressions for the change in the width are ω-dependent, however, as in the calculation of $\Delta_i{}^0$, we replace ω by the chemical potential of the system, which we take as the zero in measuring the energy.

The simplest term to understand physically is $\delta\Delta_i{}^{(2)}$, which is due to the direct transfer interaction between impurities. Naturally, $\delta\Delta_i{}^{(2)}$ is always positive and, for the simplifying condition that $E_j=0$, it is given by

$$\delta\Delta_i{}^{(2)}=\sum_{j(\neq i)}T_{ij}{}^2\frac{1}{\Delta_j{}^0}. \tag{4.6′}$$

If we assume that $T_{ij}=T$ for nearest-neighbor pair of i and j, and zero otherwise, and that $\Delta_j{}^0=\Delta^0$ independent of j, then we obtain

$$\delta\Delta_i^{(2)}/\Delta^0 = z_i(T/\Delta^0)^2, \qquad (4.6'')$$

where z_i is the number of other impurities on the nearest-neighbor sites of the ith impurity.

$\delta\Delta_i^{(1)}$ comes from the indirect interimpurity interaction through the host-metal conduction electrons. By referring to Eq. (3.15), we see $\delta\Delta_i^{(1)} \cong \pi V_j^2 \times$[the change of density of states of the host-metal conduction electrons of the Fermi surface at the ith impurity site due to the presence of other surrounding impurities]. Since the change in the host-metal density of states can be either positive or negative, $\delta\Delta_i^{(1)}$ can be either positive or negative. The possibility of $\delta\Delta_i^{(1)}$ becoming negative differentiates the behavior of $\delta\Delta_i^{(1)}$ from $\delta\Delta_i^{(2)}$. In the following, we examine $\delta\Delta_i^{(1)}$ in more detail. The calculation of the function which appears in Eq. (4.5)

$$F_R(\omega) = \sum_k \frac{e^{ikR}}{\omega - \epsilon_k + i0^+}, \qquad (4.8)$$

for a real energy band, is, in general, a very complicated task as was discussed by Koster.[38] However, for a parabolic band it is easily calculated as

$$F_R(\omega) = \frac{\Omega}{4\pi}\frac{2m}{\hbar^2}\frac{1}{R}\exp\left[i\left(\frac{2m}{\hbar^2}(\omega-\epsilon_c)\right)^{1/2} R\right], \qquad (4.8')$$

where Ω is the volume of the system and ϵ_c is the bottom of the conduction-electron band. With this simplification Eq. (4.5) reduces to

$$\delta\Delta_i^{(1)} = V_i^2\left(\frac{\Omega}{4\pi}\right)^2\left(\frac{2m}{\hbar^2}\right)^2$$
$$\times \sum_{j(\neq i)} V_j^2\left(\frac{\Delta_j^0}{(\omega-E_j)^2+\Delta_j^{02}}\right.$$
$$\times \frac{\cos\{2[(2m/\hbar^2)(\omega-\epsilon_c)]^{1/2}R_{ij}\}}{R_{ij}^2} - \frac{(\omega-E_j)}{(\omega-E_j)^2+\Delta_j^{02}}$$
$$\left.\times \frac{\sin\{2[(2m/\hbar^2)(\omega-\epsilon_c)]^{1/2}R_{ij}\}}{R_{ij}^2}\right). \qquad (4.9)$$

In Eq. (4.9), as we did for Δ_i^0, we equate ω to the Fermi energy. With this approximation and our assumption that $E_j \cong 0$, Eq. (4.9) simplifies to

$$\delta\Delta_i^{(1)} \cong V_i^2\left(\frac{\Omega}{4\pi}\right)^2\left(\frac{2m}{\hbar^2}\right)^2 \sum_{j(\neq i)} \frac{V_j^2\cos(2k_F R_{ij})}{\Delta_j^0 R_{ij}^2}, \qquad (4.10)$$

where k_F is the effective Fermi wave number of the conduction-electron band. Further, if we notice $\Delta_j^0 = \pi V_j^2 \rho_c^0(0)$, where $\rho_c^0(0) = (mk_F/2\pi^2\hbar^2)\Omega$ is the unperturbed density of states of the host metal [see Eq. (3.17)], Eq. (4.10) is reduced further:

$$\frac{\delta\Delta_i^{(1)}}{\Delta_i^0} = \frac{1}{k_F^2}\sum_{j(\neq i)}\frac{\cos(2k_F R_{ij})}{R_{ij}^2}. \qquad (4.11)$$

The oscillatory behavior of $\delta\Delta_i^{(1)}$ has the same origin as that of the well-known Ruderman-Kittel oscillation.[27,28] Note in our approximation that the difference in the species of impurities does not show up in the final result, Eq. (4.11). As is seen from Eq. (4.10) or (4.11), the effect of the surrounding impurity is most important when it is at a nearest-neighbor site. If we consider only the effect of the nearest-neighbor site impurity, assuming a simple cubic lattice, Eq. (4.11) reduces to

$$\delta\Delta_i^{(1)}/\Delta_i^0 = 4z_i\cos(2k_F d)/(2k_F d)^2, \qquad (4.11')$$

where d is the interatomic distance. Note that $\cos(2k_F d)$ varies from -1 to 1 depending upon the value of $2k_F d$. We immediately see that it is quite reasonable that $\delta\Delta_i^{(1)}/\Delta^0$ can be on the order of 0.1 by having a single other impurity in its nearest-neighbor site.

$\delta\Delta_i^{(3)}$ can be discussed in a manner quite similar to the case of $\delta\Delta_i^{(1)}$, and the magnitude of this cross term is generally in between $\delta\Delta_i^{(1)}$ and $\delta\Delta_i^{(2)}$.

It is not a simple problem to determine which change in the impurity-state width $\delta\Delta_i^{(1)}$ or $\delta\Delta_i^{(2)}$ is more important, although it has been rather customary to assume that for a nearest-neighbor pair of impurities the direct-transfer term, which gives rise to $\delta\Delta_i^{(2)}$, dominates. We know, for instance, in rare-earth metals, the indirect interaction via the conduction electrons dominates the direct interaction between a nearest-neighbor pair of localized $4f$ states. Let us try to get a crude estimate of the relative magnitudes of $\delta\Delta_i^{(1)}$ and $\delta\Delta_i^{(2)}$. From Eqs. (4.6″) and (4.11′),

$$|\delta\Delta_i^{(1)}|/\delta\Delta_i^{(2)} \cong [4/(2k_F d)^2](\Delta_i^0/T)^2. \qquad (4.12)$$

In the tight-binding approximation, the bandwidth is given by $2T$ times the number of the nearest-neighbor sites. T for the simple cubic lattice is roughly estimated to be $T \sim \frac{1}{8}W_i$, where W_i is the bandwidth of the d electrons if the impurities we are considering are transition-metal elements. On the other hand, the host-metal density of states can be expressed in terms of the host-metal bandwidth W_c as $\sim N/W_c$, thus, $\Delta_i^0 \cong \pi V^2 N/W_c$. Putting these estimates into Eq. (4.12) and replacing $2k_F d$ by π, Eq. (4.12) reduces to

$$|\delta\Delta_i^{(1)}|/\delta\Delta_i^{(2)} \cong 4\times 8^2(V^2N/W_cW_i)^2. \qquad (4.12')$$

In Eq. (4.12′), $W_i \cong$ the $3d$ bandwidth $\cong 4 \approx 6$ eV. If the host metal is also a transition metal, as in the cases of Jaccarino and Walker,[14] we may assume $W_c \cong W_i \cong 5$ eV. The last quantity we need to estimate is $V\sqrt{N}$. Note that in our normalization[24] $V\sqrt{N}$ is the quantity on the order of the one-particle energy and generally it is assumed to vary between 1 and 2 eV. The magnitude of the Eq. (4.12) can be either bigger or less than 1,

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[38] G. F. Koster, Phys. Rev. 95, 1436 (1954).

depending upon the value for $V\sqrt{N}$:

$$\frac{|\delta\Delta_i^{(1)}|}{\delta\Delta_i^{(2)}}=4\times 8^2\left(\frac{1^2}{5^2}\right)^2\cong 0.41\,,\ \text{for } V\sqrt{N}=1\text{ eV}$$
$$=4\times 8^2\left(\frac{2^2}{5^2}\right)^2\cong 6.6\,,\ \text{for } V\sqrt{N}=2\text{ eV}\,. \qquad (4.12'')$$

From the above discussion, it seems quite reasonable to assume the possibility of either case A, $|\delta\Delta_i^{(1)}|\gg\delta\Delta_i^{(2)}$, or B, $|\delta\Delta_i^{(1)}|\ll|\delta\Delta_i^{(2)}|$. In both cases, $\delta\Delta_i^{(3)}$ may be neglected compared with the dominant term.

Case A is most interesting, since in this limit $\delta\Delta_i\cong\delta\Delta_i^{(1)}$ can be negative as well as positive. Therefore, we have the possibility of explaining case I, Eq. (4.1), or case I′, Eq. (4.1′), of the local-environment effect, as well as case II. In case B, $\delta\Delta_i\cong\delta\Delta_i^{(2)}$ is always positive and only case II, Eq. (4.2), of the local-environment effect, is possible.

In the following, we discuss the historical experiment[14] of Co in $\mathrm{Rh}_{1-x}\mathrm{Pd}_x$ assuming case A. According to Jaccarino and Walker,[14,15] Co does not have a localized moment when all the nearest-neighbor sites of Co are occuppied by the Rh host-metal atom. We can assume, for instance,

$$U_{\mathrm{Co}}/\pi\Delta_{\mathrm{Co}}^0\cong 0.9\,. \qquad (4.13)$$

Since Co has a moment when two or more of its nearest-neighbor sites are occupied by a Pd impurity, the following inequality should be satisfied, with $z_i\geqq 2$:

$$U_{\mathrm{Co}}/\pi(\Delta_{\mathrm{Co}}^0+\delta\Delta_{\mathrm{Co}})\geqq 1\,. \qquad (4.14)$$

Using Eqs. (4.13) and (4.11′), our condition Eq. (4.14) reduces to

$$8\frac{\cos 2k_Fd}{(2k_Fd)^2}\leq-\frac{1}{10}\leq 4\frac{\cos 2k_Fd}{(2k_Fd)^2}\,. \qquad (4.14')$$

The values of k_Fd necessary to satisfy Eq. (4.14′) are $1.60<2k_Fd<1.64$, or, $4.25<2k_Fd<4.46$. Typically, k_Fd is on the order of π. Although our estimate is quite crude, the values required for k_Fd are not unreasonable.

In the above case, $\delta\Delta$ was negative, but in the case of V in Au, for instance, a positive $\delta\Delta$ would be required. Obviously, the case of V in Au can be understood in the same way as above.

Finally, we should mention that there is still another possible mechanism of a local-enviromnent effect which may be equally important. In short, the discussion in this section is based on the local-environment dependence of the imaginary part of the interaction energy $\Sigma_i(\omega)$, Eq. (4.3). The real part of the interaction energy also depends upon the local environment and should be included in the treatment of the problem, as will be shown fully in Sec. V. Although in this paper we do not discuss the second mechanism of the local-environment effect in any detail, its basic effects are included in the formulation given in Sec. V.

V. FERROMAGNETISM AND LOCAL MOMENT

In this section, we discuss the nature of the ferromagnetism in alloys like PdNi. Below a critical impurity concentration, these alloys are not ferromagnetic at any temperature and the impurity does not have a localized moment. Therefore, we start by assuming that, in the single-impurity limit, the impurity does not have a localized moment. We discuss how the ferromagnetism of an alloy is produced as we increase the impurity concentration. We are also interested in the possible relation between the onset of the ferromagnetism of the alloy and the formation of a localized moment on the impurity.

In Sec. IV, we followed the traditional approach in discussing the formation of a localized magnetic moment by considering the divergence of the magnetic susceptibility of the impurity. Similarly, the ferromagnetism of the total system is understood to occur when the total magnetic susceptibility calculated for the paramagnetic state diverges. In this section, we calculate the magnetic susceptibilities of both the impurity and the host metal electrons, including the effect of interactions between the impurity and the host, among the impurities, and among the host-metal electrons. In the discussion of the local-environment effect in Sec. IV, we used a magnetic susceptibility for the impurity which included some effects of the interaction with the other impurities but did not include all the interaction effects completely. In Sec. IV, we included only that part of the interaction effect which is responsible for the change in the impurity density of states. If we include all of these interactions mentioned above, the magnetic susceptibilities of the host-metal electrons and the impurity are not independent of each other and we have to solve a set of coupled equations for the impurity susceptibility and the host-metal susceptibility. First, we start from the impurity susceptibility and see how it couples to the host-metal susceptibility, and then we repeat the same for the host-conduction-electron susceptibility.

If we apply a magnetic field H in the direction of the z axis, the impurity state and the host-metal conduction band are magnetized. Namely, the occupation number of the ith impurity state $N_{i\pm}$ and that of the host metal $n_\pm$, which were introduced in Sec. III, are different for different spins:

$$N_{i\pm}\equiv N_i\mp\Delta N_i\,, \qquad (5.1)$$

$$n_\pm\equiv n\mp\Delta n\,. \qquad (5.2)$$

The magnetic susceptibilities for the impurity χ_i and the host metal χ_c are defined as

$$\chi_i=\mu_B(N_{i-}-N_{i+})/H=2\mu_B\Delta N_i/H\,, \qquad (5.3)$$

$$\chi_c=\mu_B(n_--n_+)/H=2\mu_B\Delta n/H\,, \qquad (5.4)$$

where we assumed the g factors of the impurity state and the host metal are the same and equal to 2. Our problem is to calculate $N_{i\pm}$ and $n_{\pm}$ by using the Green's functions obtained in Sec. III.

A. Impurity Susceptibility

Let us first calculate the impurity susceptibility. ΔN_i in Eq. (5.3) is calculated from the prescription in Eq. (3.1) using Eq. (3.14),

$$\begin{aligned} N_{i-}-N_{i+}&=2\Delta N_i \\ &=-\frac{1}{\pi}\int_{-\infty}^{\infty} f(\omega)d\omega\,\mathrm{Im}(\langle d_{i-}|d_{i-}^{\dagger}\rangle_{\omega+i0^+} \\ &\qquad -\langle d_{i+}|d_{i+}^{\dagger}\rangle_{\omega+i0^+}) \\ &=\frac{2}{\pi}\int_{-\infty}^{\infty} f(\omega)d\omega\,\mathrm{Im}(\langle d_{i+}|d_{i+}^{\dagger}\rangle_{\omega+i0^+} \\ &\qquad -\langle d_{i+}|d_{i+}^{\dagger}\rangle_{\omega+i0^+}|_{H=0})\,. \end{aligned} \tag{5.5}$$

The last equation in Eq. (5.5) is valid in the linear approximation with respect to the external magnetic field H.

If we maintain the approximation of a Lorentzian density of states for the impurity state, in general, the external field does two things: (1) It spin splits the impurity state, and (2) it changes the width of the impurity state. Fortunately, in the calculation of the linear magnetic susceptibility, the second effect, the magnetic field dependence of the width of the impurity state, does not enter at all. Therefore, for the calculation of the susceptibility, Eq. (3.14) can be rewritten as

$$\begin{aligned} \langle d_{i\pm}|d_{i\pm}^{\dagger}\rangle_{\omega}=[\omega-E_{i\pm}^{0}-U_iN_{i\mp}-V_i^2I_{c\pm}^{0}(\omega) \\ -\delta E_{i\pm}(\omega)+i\Delta_i]^{-1}, \end{aligned} \tag{5.6}$$

where $\Delta_i=\Delta_i^0+\delta\Delta_i$ as was defined in Sec. IV (note that it is independent of the spin). $\delta E_{i\pm}$ is the real part of the impurity-impurity interaction energy $\Sigma_{i\pm}(i\omega)$:

$$\delta E_{i\pm}=\mathrm{Re}[\Sigma_{i\pm}(\omega)]\,. \tag{5.7}$$

$\delta\Delta_i$ is given by Eq. (4.4). The functions $I_{c\pm}^{0}(\omega)$, $F_{0\pm}(\omega)$ are defined in Sec. III by Eqs. (3.17) and (3.16).

The Lorentzian approximation to the impurity state implies reducing Eq. (5.6) to

$$\langle d_{i\pm}|d_{i\pm}^{\dagger}\rangle_{\omega}=[(\omega-E_{i\pm})+i\Delta_i]^{-1}, \tag{5.8}$$

where $E_{i\pm}$ as well as Δ_i is ω-independent and

$$E_{i\pm}=E_i\pm\Delta E_i\,, \tag{5.9}$$

with $\Delta E_i\propto H$. If the impurity Green's function is of the form of Eq. (5.8), the calculation of the linear magnetization Eq. (5.5) becomes straightforward. From Eq. (5.8), the impurity density of states $\rho_i(\omega)$ is given as

$$\begin{aligned} \rho_{i\pm}(\omega)&=-(1/\pi)\,\mathrm{Im}\langle d_{i\pm}|d_{i\pm}^{\dagger}\rangle_{\omega+i0^+} \\ &=(1/\pi)\{\Delta/[(\omega-E_{i\pm})^2+\Delta^2]\}\,. \end{aligned} \tag{5.8$'$}$$

Note that, in Sec. IV, we had already assumed this form for the impurity density of states. With Eq. (5.8′), Eq. (5.5) is rewritten as

$$\begin{aligned} \Delta N_i&=-\int_{-\infty}^{\infty} f(\omega)d\omega[\rho_{i+}(\omega)|_{H}-\rho_{i+}(\omega)|_{H=0}] \\ &=\int_{-\infty}^{\infty} f(\omega)d\omega\frac{\partial}{\partial\omega}\rho_i(\omega)\Delta E_i\,, \end{aligned} \tag{5.10}$$

where $\rho_i(\omega)$ is given by Eq. (5.8′) with $E_{i\pm}$ replaced by E_i. At zero temperature, to which the discussion in this section is confined, Eq. (5.10) reduces to

$$\Delta N_i=\rho_i(0)\Delta E_i\,. \tag{5.11}$$

We must know $\rho_i(0)$, the impurity density states at the Fermi surface, and ΔE_i, the shift of the center of impurity state due to the external magnetic field. $\rho_i(0)$ was discussed in Sec. IV, and there we showed how the difference in the local environment changes $\rho_i(0)$. Therefore, the remaining problem is to obtain an explicit expression for ΔE_i.

The approximation of Eq. (5.6) by Eq. (5.8) may be realized by setting E_i and ΔE_i equal to

$$E_i=E_i^0+U_iN_i+V_i^2I_c^0(0)+\delta E_i(0)\,, \tag{5.12}$$

$$\Delta E_i=\alpha_i\mu_BH+U_i\Delta N_i+a_iv\Delta n+\sum_{j(\neq i)}c_{ij}U_j\Delta N_j\,. \tag{5.13}$$

The shift of impurity energy due to an external field consists of many terms as is given in Eq. (5.13). First, the main contribution to α_i of the Zeeman-shift term comes from the simple Zeeman shift of the impurity level. The external magnetic field Zeeman shifts the conduction electrons and a dominant part of this effect comes through the shift of the third term on the right-hand side of Eq. (5.12). Note that on the right-hand side of Eq. (5.12) $\delta E_i/V_i^2I_c^0(0)\equiv O(N_0/N\Delta/\epsilon_F)$ and, therefore, the Zeeman shift of the fourth term is of higher order than the third, especially for small impurity concentrations. Retaining only these two dominant shifts due to the Zeeman splitting,

$$\alpha_i=1-V_i^2I_c^{0\prime}(0)\,, \tag{5.14}$$

where the prime means the differentiation with respect to ω. The second term on the right-hand side of Eq. (5.13) is the exchange shift due to the molecular field of the intra-impurity Coulomb repulsion. This term was discussed in the original work of Anderson.[24] The third term on the right-hand side of Eq. (5.13) is the exchange shift due to the molecular field of the conduction electron magnetization. The dominant contribution to a_i comes from the exchange shift of the third term on the right-hand side of Eq. (5.12):

$$a_i=-V_i^2I_c^{0\prime}(0)\,. \tag{5.15}$$

The exchange shift of the fourth term in Eq. (5.12) also has a component which contributes to a_i, but we neglect it since it is of higher order than the term we retained in Eq. (5.15). The last term in Eq. (5.13) is the exchange shift due to the molecular field from the other surrounding impurities and, from Eq. (5.7), the coupling constant c_{ij} is given as

$$c_{ij}=-\mathrm{Re}\left([V_iV_jF_{ij}(0)+T_{ij}]^2 \times\left(\frac{1}{\omega-E_j^0-U_jN_j-V_j^2F_0(0)}\right)'\bigg|_{\omega=0}\right). \quad (5.16)$$

Upon substituting Eq. (5.13) into Eq. (5.11), we obtain

$$[1-U_i\rho_i(0)]\Delta N_i=\rho_i(0)(\alpha_i\mu_\beta H+a_iv\Delta n + \sum_{j(\neq i)} c_{ij}U_j\Delta N_j). \quad (5.17)$$

Now we clearly see the magnetization of the ith impurity is coupled to the magnetization of the host-metal conduction electrons (Δn) and the surrounding impurities (ΔN_j, $j\neq i$). Since $c_{ij}=0$ and $v=0$, this coupling is not present in the single-impurity limit treatment with noninteracting host-metal electrons. We briefly discuss the coupling constants a_i and c_{ij} appearing in Eq. (5.16).

The interaction between the impurity and the host metal is either ferromagnetic or antiferromagnetic, depending upon whether the sign of a_i, Eq. (5.15), is either positive or negative. Fortunately, the quantity a_i can be rather easily estimated. In Fig. 1, we sketch a typical behavior of $I_c^0(\omega)$ for a parabolic conduction-electron density of states $\rho_c^0(\omega)$. [Notice that a similar behavior is observed for a Lorentzian density of states (see Fig. 2).] From this Fig. 1, we see that a_i $[\propto -I_c^{0\prime}(0)]>0$ (ferromagnetic) when the host-metal conduction band is nearly empty or nearly filled and $a_i<0$ otherwise. The magnitude of a_i is on the order of Δ_0/ϵ_F. In Pd, for example, where we are referring to $4d$ electrons as the host-metal electrons, the band is almost filled, and a_i is likely to be positive. For actual transition metals, the band structure is not as simple as shown in Fig. 1, and accordingly, a quantitative estimate of a_i is not simple.

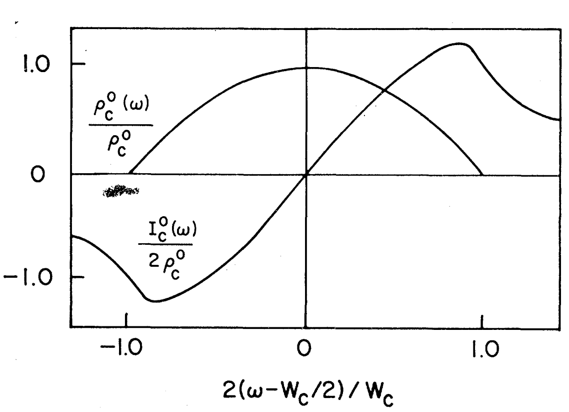

FIG. 1. The behavior of $I_c^0(\omega)$ for a parabolic density of states for the conduction electrons $\rho_c^0(\omega)=\rho_c^0\{1-[(\omega-\frac{1}{2}w_c)/\frac{1}{2}w_c]^2\}$.

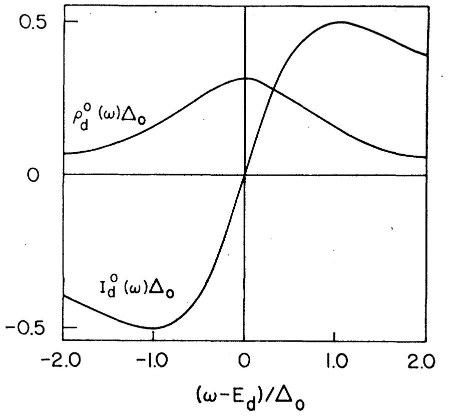

FIG. 2. The behavior of $I_d^0(\omega)$ for a Lorentzian density of states of an impurity $\rho_d^0(\omega)=(1/\pi)\{\Delta_0/[(\omega-E_d)^2+\Delta_0^2]\}$. Note that the relation between $\rho_d^0(\omega)$ and $I_d^0(\omega)$ shown here can be regarded as a relation between $\rho_c^0(\omega)$ and $I_c^0(\omega)$ for a Lorentzian density of states for the conduction electrons.

The interimpurity coupling constant c_{ij} consists of three different components:

$$c_{ij}=c_{ij}^{(1)}+c_{ij}^{(2)}+c_{ij}^{(3)}, \quad (5.18)$$

$$c_{ij}^{(1)}=-\mathrm{Re}\left[V_i^2V_j^2F_{ij}(0)^2 \times\left(\frac{1}{\omega-E_j^0-U_jN_j-V_j^2F_0(0)}\right)'\bigg|_{\omega=0}\right], \quad (5.19)$$

$$c_{ij}^{(2)}=-T_{ij}^2\,\mathrm{Re}\left[\left(\frac{1}{\omega-E_j^0-U_jN_j-V_j^2F_0(0)}\right)'\bigg|_{\omega=0}\right] =-T_{ij}^2I_j^{0\prime}(0), \quad (5.20)$$

$$c_{ij}^{(3)}=-2V_iV_jT_{ij} \times\mathrm{Re}\left[F_{ij}(0)\left(\frac{1}{\omega-E_j^0-U_jN_j-V_j^2F_0(0)}\right)'\bigg|_{\omega=0}\right]. \quad (5.21)$$

The decomposition of c_{ij}, Eq. (15.18), exactly corresponds to the previous decomposition of $\delta\Delta_i$, Eq. (4.4). In Eq. (5.20), $I_j^0(\omega)$ is introduced as the real part of the jth impurity Green's function in the single-impurity limit. [Previously, in Sec. IV, we introduced the corresponding imaginary part, $-\pi\rho_j^0(\omega)$.] Let us briefly discuss these three components of c_{ij}.

The term $c_{ij}^{(2)}$ originates from the direct transfer between impurities and is the simplest to understand, as was the corresponding term $\delta\Delta_i^{(2)}$ in Sec. IV. We consider a nearest-neighbor pair of identical impurities, for which

$$c_{ij}^{(2)}=-T^2I_j^{0\prime}(0)=-T^2I_i^{0\prime}(0). \quad (5.22)$$

In Fig. 2, we show the general characteristic of $I_i^0(\omega)$

corresponding to a Lorentzian density of states for the impurity $\rho_i^0(\omega)$. From Eq. (5.22) and Fig. 2, we can immediately draw the following conclusions for a nearest-neighbor pair of localized impurity states: (1) When the localized (impurity) state is nearly half filled $c_{ij}^{(2)}$ is negative and, therefore, the interaction is antiferromagnetic. (2) When the localized state is nearly filled or almost empty, $c_{ij}^{(2)}$ is positive and, therefore, the interaction is ferromagnetic. These conclusions can be extended to the more general case where the pair of nearest-neighbor localized states are of different species. It is interesting to note that the two conclusions above though obtained from a very simple treatment are essentially the same as the conclusion of Moriya.[30]

The term $c_{ij}^{(1)}$ results from the indirect coupling of the impurities through the conduction electrons. As in Sec. IV, if we assume Eq. (4.8′), which is valid for a parabolic conduction band, $c_{ij}^{(1)}$ is explicitly given by

$$c_{ij}^{(1)}=V_i^2V_j^2\left(\frac{\Omega}{4\pi}\right)^2\left(\frac{2m}{\hbar^2}\right)^2\frac{1}{R_{ji}^2}$$
$$\times\{\cos(2k_FR_{ij})[I_j^0(0)^2-\pi^2\rho_j^0(0)^2]$$
$$-\sin(2k_FR_{ij})2\pi I_j^0(0)\rho_j^0(0)\}. \quad (5.23)$$

If we assume that the ith and jth impurities are of the same kind and the impurity states are nearly half filled, $E_i=E_j\cong 0$, and Eq. (5.23) simplifies to

$$c_{ij}^{(1)}=-4\cos(2k_FR_{ij})/(2k_FR_{ij})^2. \quad (5.23')$$

To obtain the relative importance of $c_{ij}^{(1)}$ versus $c_{ij}^{(2)}$ from Eq. (5.22) and (5.23′), the same discussion as presented for $\delta\Delta^{(1)}$ versus $\delta\Delta^{(2)}$ holds.

The term $c_{ij}^{(3)}$ is a result of the cross effect of the two processes discussed in the above and, therefore, its magnitude is generally intermediate between $c_{ij}^{(1)}$ and $c_{ij}^{(2)}$.

B. Host-Metal Susceptibility

We proceed to calculate the magnetization of the conduction electrons:

$$(n_--n_+)=2\Delta n$$
$$=-\frac{1}{\pi}\operatorname{Im}\int_{-\infty}^{\infty}f(\omega)d\omega\Big(\sum_k\langle c_{k-}|c_{k-}^\dagger\rangle_{\omega+i0^+}$$
$$-\sum_k\langle c_{k+}|c_{k+}^\dagger\rangle_{\omega+i0^+}\Big), \quad (5.24)$$

where, from Eq. (3.15),

$$\sum_k\langle c_{k\pm}|c_{k\pm}^\dagger\rangle_\omega=F_{0\pm}(\omega)-F_{0\pm}'(\omega)\sum_i V_i^2\langle d_{i\pm}|d_{i\pm}^\dagger\rangle_\omega$$
$$-\sum_{i\neq j}V_iV_j[V_iV_jF_{ij\pm}(\omega)+T_{ij}]F_{ij\pm}'(\omega)\langle d_{i\pm}|d_{i\pm}^\dagger\rangle_\omega$$
$$\times\frac{1}{\omega-E_{j\pm}^0-U_jN_{j\mp}-V_j^2F_{0\pm}(\omega)}. \quad (5.25)$$

In carrying out the program Eq. (5.24), we neglect the third term on the right-hand side of Eq. (5.25) for the following reasons. First, the third term represents the perturbation of the conduction electron which is quadratic in the impurity concentration, whereas the second term which is retained is linear in the impurity concentration. Therefore, this simplification is justifiable particularly for the low-impurity-concentration region. Second, in calculating the magnetization, we obtain all of the physically interesting terms which are proportional to H, Δn, and ΔN_i from the first two terms on the right-hand side of Eq. (5.25). Therefore, the inclusion of the third term is only of quantitative importance. By expanding the integrands in Eq. (5.24) in terms of H, Δn, and ΔN_i, we obtain

$$\Delta n=\mu_B\rho_{c1}(0)H+v\rho_{c2}(0)\Delta n$$
$$+\frac{1}{N}\sum_i b_i\rho_{c1}(0)U_i\Delta N_i, \quad (5.26)$$

$$\rho_{c1}(0)=\rho_c^0(0)-\sum_i V_i^2(\langle\langle\rho_iI_c^{0\prime\prime}\rangle\rangle+\langle\langle I_i\rho_c^{0\prime\prime}\rangle\rangle)$$
$$-\sum_i V_i^2[1-V_i^2I_c^{0\prime}(0)]$$
$$\times(\langle\langle I_c^{0\prime}\rho_i'\rangle\rangle+\langle\langle\rho_c^{0\prime}I_i'\rangle\rangle), \quad (5.27)$$

$$\rho_{c2}(0)=\rho_c^0(0)-\sum_i V_i^2(\langle\langle\rho_iI_c^{0\prime\prime}\rangle\rangle+\langle\langle I_i\rho_c^{0\prime\prime}\rangle\rangle)$$
$$+\sum_i V_i^4I_c'(0)(\langle\langle I_c^{0\prime}\rho_i'\rangle\rangle+\langle\langle\rho_c^{0\prime}I_i'\rangle\rangle), \quad (5.28)$$

$$(1/N)b_i\rho_{c1}(0)\equiv V_i^2(\langle\langle I_c^{0\prime}\rho_i'\rangle\rangle+\langle\langle\rho_c^{0\prime}I_i'\rangle\rangle), \quad (5.29)$$

where $I_c^0(\omega)$ and $\rho_c^0(\omega)$ are defined in Eq. (3.17), $I_i(\omega)$ is the real part of the ith impurity Green's function Eq. (5.8), $\rho_i(\omega)$ is defined in Eq. (5.8′), with $H=0$, and the notation $\langle\langle\cdots\rangle\rangle$ means

$$\langle\langle g\rangle\rangle=\int_{-\infty}^{\infty}f(\omega)g(\omega)d\omega \quad (5.30)$$

$$\cong\int_{-\infty}^{\epsilon_F}g(\omega)d\omega. \quad (5.30')$$

In Eq. (5.30), $f(\omega)$ is the Fermi distribution function and in this section we always adopt the zero-temperature limit Eq. (5.30′).

Notice that both $\rho_{c1}(0)$ and $\rho_{c2}(0)$ are slightly different from the real perturbed density of states of the host metal $\rho_c(0)$, which is obtained by simply taking the imaginary part of the Eq. (5.25) at $H=0$. In the same approximation as Eqs. (5.27) and (5.28), $\rho_c(0)$ is given as

$$\rho_c(0)=\rho_c^0(0)-[\rho_c^{0\prime}(0)\sum_i V_i^2I_i(0)+I_c^{0\prime}(0)\sum_i V_i^2\rho_i(0)].$$

ρ_c, ρ_{c1}, and ρ_{c2} become equal in the case of simple potential scattering where the quantity corresponding to $\langle d_{i\pm}|d_{i\pm}^\dagger\rangle_\omega$ in Eq. (5.25) or (3.15) is a constant independent of ω.

C. Coupled Equations of χ_i and χ_c

Equations (5.17) and (5.26) represent a set of coupled equations for ΔN_i and Δn. We rewrite these equations for ΔN_i and Δn in terms of the impurity- and host-metal susceptibilities [see Eqs. (5.3) and (5.4)]:

$$\chi_i=\alpha_i\chi_i^0+a_iv\chi_i^0\chi_c+\chi_i^0\sum_{j(\neq i)}c_{ij}U_j\chi_j, \tag{5.31}$$

$$\chi_c=\chi_c^0+\frac{1}{N}\chi_c^0\sum_j b_jU_j\chi_j, \tag{5.32}$$

where we have temporarily set $2\mu_B^2=1$, and

$$\chi_i^0\equiv\rho_i(0)/[1-U_i\rho_i(0)], \tag{5.33}$$

$$\chi_c^0\equiv\rho_{c1}(0)/[1-v\rho_{c2}(0)]. \tag{5.34}$$

We assume χ_i^0's and χ_c^0 are not diverging (and positive).

From these coupled equations, Eqs. (5.31) and (5.32), we can make the general observation that *all the three magnetic susceptibilities* χ_i, $\sum_i\chi_i$, *and* χ_c, *diverge at the same time, i.e., the condition for the occurrence of a localized magnetic moment on an impurity is identical with that for the ferromagnetism of the impurity system and the ferromagnetism of the host-metal conduction electrons.* Usually, local-moment formation is associated with the divergence of χ_i, without divergence in χ_c. This situation is impossible if the interactions between the impurity and the host, among the impurities, and among the host electrons are properly taken into account.

From Eq. (5.31), it is easy to see that χ_i is proportional to χ_i^0. This fact justifies our discussion on the local-environment effects in Sec. IV which was based on χ_i^0 and not on the real impurity susceptibility χ_i. For the magnetized state, the impurities do not behave identically. Those impurities, for which χ_i^0 are discontinuously larger than other impurities, will have a larger net magnetic moment in the magnetized state.

From Eq. (5.31), however, we note that there is still another source of the local-environment effect besides the first one which is included in χ_i^0. Namely, the contribution of the last term on the right-hand side of Eq. (5.31) depends upon the distribution of the surrounding impurities. As is well known, if we use the simple molecular field approximation in solving Eqs. (5.31) and (5.32), however, this second kind of local-environment effect will not be retained. In this paper, we do not try to consider this second mechanism of the local-environment effect, although it may be as important as the local-environment effect contained in χ_i^0.

If the Coulomb interaction between the host-metal electrons v is sufficiently strong (say, $v\chi_c^0\gg1$) as in the metal Pd, the long-range interimpurity interaction through the second term on the right-hand side of Eq. (5.31) will be dominant over the last term on the right-hand side of Eq. (5.31). Since in this paper we are particularly interested in Pd alloys, we solve the coupled equations, Eqs. (5.31) and (5.32), only for this limiting case by neglecting the last term on the right-hand side of Eq. (5.31). For this case (i.e., $c_{ij}=0$), the coupled equations are easily solved:

$$\chi_i=\chi_i^0\frac{1}{\mathrm{CD}}\left(\alpha_i+a_iv\chi_c^0+v\chi_c^0\times\frac{1}{N}\sum_j(\alpha_ja_i-\alpha_ia_j)b_jU_j\chi_j^0\right), \tag{5.35}$$

$$\chi_c=\chi_c^0\frac{1}{\mathrm{CD}}\left(1+\frac{1}{N}\sum_j\alpha_jb_jU_j\chi_j^0\right), \tag{5.36}$$

where the common denominator (CD) of the susceptibilities is

$$\mathrm{CD}=1-\frac{1}{N}\sum_j a_jb_j(v\chi_c^0)(U_j\chi_j^0). \tag{5.37}$$

If there is only one kind of impurity, we can drop the suffix i from U_i, α_i, and a_i and neglect the weak i dependence of b_i. Then, Eqs. (5.35), (5.36), and (5.37) reduce to

$$\chi_i=\chi_i^0(1/\mathrm{CD})(\alpha+av\chi_c^0), \tag{5.35$'$}$$

$$\chi_c=\chi_c^0\frac{1}{\mathrm{CD}}\left(1+\frac{1}{N}U\alpha b\sum_j\chi_j^0\right), \tag{5.36$'$}$$

$$\mathrm{CD}=1-abv\chi_c^0U\frac{1}{N}\sum_j\chi_j^0. \tag{5.37$'$}$$

From those explicit solutions, we reconfirm our previous observation. First, χ_i, $\sum_i\chi_i$, and χ_c diverge together if and only if the common denominator Eq. (5.37) or (5.37′) vanishes. Second, χ_i is proportional to χ_i^0 and, therefore, the local enivronment effect is included through χ_i^0.

As we have previously stated, the explicit solution has been obtained only for the case in which the Coulomb interaction between the host-metal electrons is strong and, accordingly, the interimpurity interaction arising from the second term dominates the third term on the right-hand side of Eq. (5.31). The general structure of our solution Eqs. (5.35) or (5.36) with a common denominator, however, is expected to be valid beyond this restriction.

Now the condition for the ferromagnetism of the total system is given by

$$\mathrm{CD}=0. \tag{5.38}$$

Since χ_c^0 and χ_j^0 are positive, the necessary (but not sufficient) condition for the realization of the condition in Eq. (5.38) is, for the simple case of Eq. (5.37′),

$$ab>0. \tag{5.39}$$

If the condition Eq. (5.39) is satisfied, we can realize Eq. (5.38) by either increasing the impurity concentration or lowering the temperature to increase χ_j^0 (or χ_c^0). If, however, Eq. (5.39) is not satisfied and

$$ab<0, \tag{5.40}$$

the condition Eq. (5.38) can never be satisfied and the alloy cannot become ferromagnetic. Therefore, in our theory, the signs of the quantities a and b are of crucial importance. The nature of the quantity a is rather simple as is seen from Eq. (5.15). The quantity b, defined in Eq. (5.29), is more complicated. Although in a later publication we plan to estimate this quantity numerically for a simplified model, here we only mention that b, as well as a, can be either positive or negative and its magnitude is $O(1)$. A very crude estimation of the sign of b can be obtained using Figs. 1 and 2.

It should be noted that in the whole discussion of this section we have implicitly assumed that all the χ_i^0's are finite. Due to the local environment effects, as discussed in Sec. IV, in certain cases some of the χ_i^0's may diverge even if in the single-impurity limit the impurity does not have a localized moment. For such a situation, the discussion in this section might have to be modified. For instance, for an alloy in which some of the χ_i^0's are diverging, a more appropriate treatment might be one which assumes the presence of a localized moment on those impurities from the start.[27–31]

In Sec. VI, we present a few examples, by analyzing the experimental data in terms of the result obtained in this section.

VI. ILLUSTRATIVE EXAMPLES

In this section, we discuss a few ferromagnetic transition metal alloys, such as PdNi and PdRh, based on the results obtained in the previous sections for the alloys in which the host metals are strongly exchange enhanced. In order to make the discussion simple, we ignore the fact that each impurity has a different local environment, set

$$\chi_i^0=\chi_d^0 \quad \text{for all } i, \tag{6.1}$$

and assume it is positive and finite. The common denominator of the susceptibilities, Eq. (5.37′), can then be written as

$$\mathrm{CD}=1-xab(v\chi_c^0)(U\chi_d^0), \tag{6.2}$$

where $x=N_0/N$ is the impurity concentration. Further, although it is not esssential, we approximate $\alpha=1-V^2I_c^{0\prime}$ by 1. Then, from Eqs. (5.35′) and (5.36′),

$$\sum_i \chi_i=N_0\chi_d^0\frac{1}{\mathrm{CD}}(1+av\chi_c^0), \tag{6.3}$$

$$\chi_c=\chi_c^0\frac{1}{\mathrm{CD}}(1+xUb\chi_d^0). \tag{6.4}$$

As briefly mentioned at the end of Sec. V, the crucial problem is to estimate the two quantities a and b which are defined, respectively, in Eqs. (5.15) and (5.29). Generally, there may be four cases: (1) $a>0$, $b>0$ (ferromagnetic); (2) $a<0$, $b<0$ (antiferromagnetic); (3) $a>0$, $b<0$ (nonmagnetic); (4) $a<0$, $b>0$ (nonmagnetic). As is seen from Eqs. (5.13) and (5.26) in case 1, the interaction between the host-metal conduction electrons and the impurity electrons are ferromagnetic, namely, they tend to magnetize in a parallel manner.

In case 2, if $|a|v\chi_c^0>1$, which is quite possible, then χ_d is negative. As for χ_c, as long as $xU|b|\chi_d^0<1$, it is positive. In this situation, the condution electrons magnetize in the direction of the external field, whereas the impurity spins magnetize in the direction opposite to the external field. As we increase the impurity concentration x, the numerator of χ_c, which is positive for small x, as well as the CD, decreases. If $|a|v\chi_c^0>1$ as we have assumed, the CD vanishes before the numerator of χ_c changes sign and in this case the critical impurity concentration x_{crit} for antiferromagnetism is obtained from CD$=0$. If $|a|v\chi_c^0<1$ in case 2, then $\chi_d>0$ and $\chi_c>0$ for small x. However, as we increase x, the numerator of χ_c changes sign before the CD vanishes, and, therefore, from CD$=0$ we obtain again a critical impurity concentration for the occurrence of antiferromagnetism. [Note, however, that for small $v\chi_c^0$ (<1), our approximation of neglecting the last term in Eq. (5.31) is not valid.]

In cases 3 and 4, since the common denominator is always bigger than 1, χ_c and $\sum_i\chi_i$ never diverge and, therefore, no ferromagnetic or antiferromagnetic phase transition is expected.

We are most interested in case 1, since we wish to explain the behavior of the alloys such as PdNi, PdRh, and RhNi, which seem to belong to this case. In the following, we will concentrate on case 1. For these alloys, the magnetic susceptibility which is the sum of $\sum_i\chi_i$ and χ_c, Eqs. (6.3) and (6.4), can be approximated as

$$\chi_{\mathrm{alloy}}=\sum_i \chi_i+\chi_c\cong\frac{N_0\chi_d^0+\chi_c^0}{1-xab(v\chi_c^0)(U\chi_d^0)}. \tag{6.5}$$

As is easily seen, the role of the correction term in the numerator, which should be present on the right-hand side of Eq. (6.5), can be neglected compared with the role of the CD Note Eq. (6.5) is very similar to the result obtained for the s-d exchange model in which χ_d^0 is a Curie susceptibility.[32] To analyze the experimental data, we introduce two quantities from Eq. (6.5), the initial-increase rate of χ_{alloy} with the impurity concentration θ, and the critical impurity concentration for ferromagnetism x_{crit}, which is obtained from the equation CD$=0$;

$$\theta\equiv\frac{1}{\chi_c^0}\frac{d\chi_{\mathrm{alloy}}}{dx}\bigg|_{x=0}=ab(v\chi_c^0)(U\chi_d^0)+\frac{N\chi_d^0}{\chi_c^0}, \tag{6.6}$$

$$x_{\mathrm{crit}}(T)=[ab(v\chi_c^0)(U\chi_d^0)]^{-1}. \tag{6.7}$$

Note if the first term dominates the second term on the right-hand side of Eq. (6.6), x_{crit} is just the reciprocal of the initial increasing rate of χ_{alloy}, and in this limit Eqs. (6.6) and (6.7) are very similar to the result of Engelsberg, Brinkman, and Doniach[34] based on the model of Lederer and Mills.[33] As seen from Eq. (6.7), x_{crit} is temperature-dependent. The temperature dependence comes mainly from the temperature dependence of χ_d^0 and χ_c^0. Therefore, Eq. (6.7) or $\text{CD}=0$ also serves as an equation to determine the Curie temperature for a given impurity concentration. In the discussion which follows, when we refer to the experiment, it is always assumed to be at the zero-temperature limit.

In $\text{Ni}_x\text{Pd}_{1-x}$, according to the experiment,[4] θ of χ_{alloy} is ~ 87. Then from Eqs. (6.6) and (6.7), x_{crit} should equal $[87—N\chi_d^0/\chi_c^0]^{-1}$. To reproduce the experimental value of $x_{\text{crit}} \cong 2$ at.% we would have to assume $N\chi_d^0/\chi_c^0 \cong 40$. This value for χ_d^0 seems to be too large to be consistent with other experimental evidence such as the lack of a sharp magnetic field dependence of the magnetic susceptibility,[7] and the low-temperature specific heats.[4]

Another interesting system is $\text{Pd}_{1-x}\text{Rh}_x$. This system often has been treated as a typical case of the rigid-band model. Recently, some experimental evidence[39] against the simple rigid-band behavior was presented and it seems that the use of simple rigid-band models for interpreting the electronic structure of alloys is being seriously questioned. We can discuss $\text{Pd}_{1-x}\text{Rh}_x$ alloy from the same point of view as the $\text{Pd}_{1-x}\text{Ni}_x$ alloy. We treat Rh in Pd as a localized impurity state. As we put Rh into Pd, the χ_{alloy} increases and $\theta \sim 28$.[40] From Eqs. (6.6) and (6.7), and assuming $N\chi_d^0/\chi_c^0$ is on the order of 1, x_{crit} should be ~ 3 at.%. Unlike PdNi, the PdRh alloy never becomes ferromagnetic, however, and at $x \approx 5$ at.% the alloy susceptibility has a maximum and decreases thereafter.

The failure of the simple use of Eqs. (6.6) and (6.7) in correlating the observed initial increase in the magnetic susceptibility and the critical impurity concentration in PdNi and PdRh can be resolved using our theory. χ_c^0 and χ_d^0 which appear in the CD, Eq. (6.2), have a dependence on the impurity concentration. From Eqs. (5.33) and (5.34), the densities of states appearing in χ_c^0 and χ_d^0 are distorted by the presence of finite concentration x of impurities. This additional impurity concentration dependence of χ_{alloy} through χ_c^0 and χ_d^0 resolves the difficulty.

In Sec. IV, we discussed how $\rho_i(0)$ appearing in χ_i^0 is modified from $\rho_i^0(0)$. In this section, we have been assuming $\chi_i^0=\chi_d^0$, independent of the impurity site i, which implies $\rho_i(0)\equiv\rho_d(0)$, independent of the i. Since we supposed only one kind of impurities are present in the system, in the single-impurity limit, each impurity state is the same: $\rho_i^0(0)\equiv\rho_d^0(0)$, independent of i. By taking the average of the effect of the surrounding impurities over the random distribution of the impurities, $\rho_d(0)$ can be written in the form (see Appendix)

$$\rho_d(0) \cong \rho_d^0(0)(1+\gamma x), \tag{6.8}$$

for small x. Here γ is a constant whose magnitude is on the order of 1. Using Eq. (6.8), χ_d^0 is given as

$$\chi_d^0 \cong \frac{\rho_d^0(0)}{1-U\rho_d^0(0)}\left[1+\left(\frac{1}{1-U\rho_d^0(0)}+1\right)\gamma x\right]. \tag{6.9}$$

For $[1-U\rho_d^0(0)]^{-1} \gg 1$, which seems to be the case in PdNi or PdRh,

$$\chi_d^0 \cong \chi_d^{00}\{1+[\gamma/1-U\rho_d^0(0)]x\}, \tag{6.9$'$}$$

where χ_d^{00} is the real single-impurity-limit magnetic susceptibility of an impurity[24] and obtained from χ_d^0 by replacing $\rho_d(0)$ with $\rho_d^0(0)$. Equation (6.9′) corresponds to taking into account the x dependence of $\rho_d(0)$ only in the denominator of χ_d^0.

Similarly, for χ_c^0, Eq. (5.34), we obtain

$$\chi_c^0 \cong \frac{\rho_c^0(0)}{1-v\rho_{c2}(0)} \cong \chi_c^{00}\left(1+\frac{\delta}{1-v\rho_c^0(0)}x\right), \tag{6.10}$$

where δ is defined by

$$\rho_{c2}(0) \cong \rho_c^0(0)(1+\delta x) \tag{6.11}$$

(see Appendix) and is a constant whose magnitude is on the order of 1. χ_c^{00} (apart from a factor $2\mu_B^2$) is the magnetic susceptibility of the host metal without any impurities: $\chi_c^{00}=\rho_c^0(0)/[1-v\rho_c^0(0)]$. We have assumed χ_d^{00}, as well as χ_c^{00}, are finite.

Substituting Eqs. (6.9′) and (6.10) into the equation $\text{CD}=0$, we obtain an equation for the critical concentration which is quadratic in x:

$$1-xab(v\chi_c^{00})(U\chi_d^{00})\left[1+x\left(\frac{\gamma}{1-U\rho_d^0(0)}+\frac{\delta}{1-v\rho_c^0(0)}\right)\right]=0. \tag{6.12}$$

Correspondingly, the expression for the initial increase rate of the alloys susceptibility, Eq. (6.6), is modified to

$$\theta=\frac{1}{\chi_c^{00}}\frac{d\chi_{\text{alloy}}}{dx}\bigg|_{x=0}=ab(v\chi_c^{00})(U\chi_d^{00})+\frac{N\chi_d^{00}}{\chi_c^{00}}+\frac{\delta}{1-v\rho_c^0(0)}. \tag{6.13}$$

We reanalyze the experimental data on PdNi and PdRh with the new Eqs. (6.12) and (6.13). Let us first

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[39] G. N. Rao, E. Matthias, and D. A. Shirley (unpublished).

[40] R. Doclo, S. Foner, and A. Narath, J. Appl. Phys. **40**, 1206 (1966); S. Foner and E. J. McNiff, Jr., Phys. Letters **29A**, 28 (1969).

discuss PdNi. In Pd, we choose the exchange enhancement factor of the magnetic susceptibility $[1-v\rho_c{}^0(0)]^{-1}$ to be 10 and accordingly $v\chi_c{}^{00}=9$. The exchange-enhancement factor for the impurity Ni in Pd is expected to be greater than that of pure Pd, and, therefore, we assume $[1-U\rho_d{}^0(0)]^{-1}>10$ and $U\chi_d{}^{00}>10$. Although there remains great freedom in choosing values for the remaining parameters in Eq. (6.13), the following choice seems reasonable: $\theta=87 \cong ab(v\chi_c{}^{00})(U\chi_c{}^{00})$ by assuming the second and third terms on the right-hand side of Eq. (6.13) nearly cancels each other, which means $\delta\cong-\frac{1}{2}$ since $N\chi_d{}^{00}/\chi_c{}^{00}$ is believed to be less than 10. After having reproduced θ, to satisfy Eq. (6.12) with the experimentally observed value of $x_{\text{crit}}\cong2$ at.%, we have to assume

$$\gamma/[1-U\rho_d{}^0(0)]+\delta/[1-v\rho_c{}^0(0)]\cong-20,$$

implying $\gamma\cong-1$.

We proceed to the case of PdRh. A convenient choice is to assume $ab(v\chi_c{}^{00})(U\chi_d{}^{00})\cong20$, which is reasonable compared with the analysis in the above case of PdNi, since $U\chi_d{}^{00}$ of Ni is expected to be a few times bigger than that of Rh. In order to reproduce the experimental value of $\theta\cong28$, we have to assume

$$N\chi_d{}^{00}/\chi_c{}^{00}+\delta/[1-v\rho_c{}^0(0)]\cong8,$$

which implies that δ is positive and $\approx\frac{1}{2}$. Next, in order to explain the fact that in this system χ_{alloy} never diverges and that at $x\cong5$ at.% the χ_{alloy} has a maximum which is about twice that of the pure-Pd susceptibility, we have to assume $\gamma/[1-U\rho_d{}^0(0)]+\delta/[1-v\rho_c{}^0(0)] \cong-10$, which implies $\gamma\cong-1$. The local enhancement factor $1/[1-U\rho_d{}^0(0)]$ of the impurity Rh is considered to be larger than that of the host metal Pd.

In $\text{Rh}_{1-x}\text{Ni}_x$, according to the experiment,[8] $\theta\cong10$. This may be understood by comparison with the case of $\text{Pd}_{1-x}\text{Ni}_x$. Since the magnetic susceptibility of Rh metal is about 10 times smaller than that of Pd metal, $ab(v\chi_c{}^{00})(U\chi_d{}^{00})$ in $\text{Rh}_{1-x}\text{Ni}_x$ can be an order of magnitude smaller than in $\text{Pd}_{1-x}\text{Ni}_x$. Thus, $ab(v\chi_c{}^{00})(U\chi_d{}^{00}) <10$. Since the exchange-enhancement factor of Rh metal is ≈2, the contribution of the third term on the right-hand side of Eq. (6.13) is $\pm0(1)$. Therefore, the second term in Eq. (6.13) may contribute significantly to θ. The experimentally observed x_{crit} of Ni in Rh is ≈63 at.%. Since our whole discussion is valid in the small-impurity-concentration region, it would be incorrect to discuss x_{crit} from our Eq. (6.13). However, if we assume $abv\chi_c{}^{00}U\chi_d{}^{00}=5$ [accordingly $N\chi_d{}^{00}/\chi_c{}^{00} +\delta(1-v\rho_c{}^0(0))\cong5$ to reproduce $\theta=10$], and

$$\gamma/[1-U\rho_d{}^0(0)]+\delta/[1-v\rho_c{}^0(0)]\cong-0.76,$$

the value of $x_{\text{crit}}=63\%$ is obtained. It seems γ and δ have opposite signs and $\gamma/[1-U\rho_d{}^0(0)]$ and $\delta/[1-v\rho_c{}^0(0)]$ nearly cancel each other to make the sum rather small.

The above analysis of the experimental data is far from being unique. We should not be too critical at this stage since even in pure Pd metal, for instance, we do not have a good limit on the value of the exchange-enhancement factor in spite of a great deal of experimental and theoretical studies.[41] What is important to stress is the qualitative aspect of our result such as the nonlinear impurity concentration dependence of the denominator of the alloy susceptibility which allows us to explain various problems which have not been explained previously.

VII. CONCLUDING REMARKS

In this paper, we attempted to construct a theory of transition-metal alloys based on the Anderson model. Effort was made to consider coherently both the electronic structure and the electronic interaction. The magnetic properties of some transitoin-metal alloys are reasonably well explained by our theory. Recently, an interesting neutron scattering experiment was done on CuNi.[13] Essentially, the following two facts were observed by neutron diffraction. The first fact is that only a tiny fraction of Ni atoms play the role of polarization cloud centers. This seems to be related to the local-environment effect discussed in Sec. IV. For instance, we can assume that those Ni atoms for which all nearest-neighbor sites are Ni have discontinuously larger magnetic susceptibility than the other Ni's. Thus, in the ferromagnetic state, the central Ni atom magnetizes more easily than the other Ni's and becomes the center of a polarization cloud. Second, from the very large spatial range of this polarization cloud, we may assume that the host susceptibility is greatly exchange enhanced. This kind of behavior was also studied in this paper. Due to the interactions between the host and the impurity, in certain cases the host susceptibility can be greatly exchange enhanced. In Cu alloys, however, where the Coulomb interaction between host-metal electrons is not as big as in Pd, we should take a different approximation in handling our fundamental equations, Eqs. (5.31) and (5.32). Namely, the inter-impurity interaction through c_{ij} becomes more important than in the case of Pd alloys.

Recently, there have been very lively discussions on the nature of a localized moment in a metal. It was first assumed that a localized moment is present in an impurity (*s-d* exchange model) and then the interaction between a single localized moment and the conduction electrons was considered to higher order on the *s-d* exchange interaction (Kondo effect[42]). Similar higher-order effects in the single-impurity limit have also been

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[41] S. Foner and E. J. McNiff, Jr., Phys. Rev. Letters **19**, 1438 (1967).

[42] J. Kondo, Progr. Theoret. Phys. (Kyoto) **32**, 37 (1964). For many recent references, see M. D. Daybell and W. A. Steyert, Rev. Mod. Phys. **40** (1968).

considered using the Anderson model[43] and the Wolff model.[44] In this paper, we presented discussions for the many impurity case within the simple Hartree-Fock approximation. Those higher-order considerations made in a single-impurity limit can be included in the present discussions of the many-impurity case.

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APPENDIX: CALCULATION OF γ AND δ

Calculation of γ

By introducing the simplification of the type of Eq. (6.1) into Eq. (3.14), we obtain

$$\langle d_{i+}|d_{i+}^{\dagger}\rangle_{\omega}=[\omega-E_d^0-UN_- -V^2F_0(\omega)-\Sigma_i(\omega)]^{-1}, \quad \text{(A1)}$$

where, neglecting the direct-transfer terms for simplicity [see Eq. (4.3)],

$$\Sigma_i(\omega)=V^4\frac{1}{\omega-E_d^0-UN_- -V^2F_0(\omega)} \times\sum_{j(\neq i)}F_{ij}(\omega)F_{ji}(\omega) \quad \text{(A2)}$$

is the self-energy due to the interaction with other impurities and $F_{ij}(\omega)$ is given by Eq. (3.16). In carrying out the summation over the randomly distributed impurities in Eq. (A2), we adopt the simplest approximation,

$$\sum_{j(\neq i)}F_{ij}(\omega)F_{ji}(\omega)\cong\frac{N_0}{N}\sum_{j,\text{ all lattice points}}{}^{'}F_{0j}F_{j0}, \quad \text{(A3)}$$

where the prime on the summation indicates to exclude $j=0$ from the summation. From Eqs. (A2) and (A3),

$$\Sigma_i(\omega)=\frac{N_0}{N}V^4\frac{1}{\omega-E_d^0-UN_- -V^2F_0(\omega)} \times[-NF_0'(\omega)-F_0(\omega)^2]. \quad \text{(A4)}$$

Note that $\Sigma_i(\omega)$, which now is independent of i, is proportional to the impurity concentration $x=N_0/N$.

For the small impurity concentration limit, Eq. (A1) may be expanded as

$$\begin{aligned}\langle d_{i+}|d_{i+}^{\dagger}\rangle_{\omega}&=G_{d+}^0(\omega)+\Sigma_i(\omega)[G_{d+}^0(\omega)]^2+\cdots\\&=G_{d+}^0(\omega)+xV^4[G_{d+}^0(\omega)]^3\\&\qquad\times[-NF_0'(\omega)-F_0(\omega)^2]+\cdots, \quad \text{(A5)}\end{aligned}$$

where for brevity we introduced

$$G_{d+}^0(\omega)=1/[\omega-E_d^0-UN_- -V^2F_0(\omega)]. \quad \text{(A6)}$$

By a procedure similar to Eq. (5.8′), we obtain from Eq. (A5)

$$\rho_d(\omega)=\rho_d^0(\omega)+xV^4\left(-\frac{1}{\pi}\right) \times\text{Im}\{[G_{d+}^0(\omega)]^3[-NF_0'(\omega)-F_0(\omega)^2]\} \quad \text{(A7)}$$

or γ, defined in Eq. (6.8),

$$\gamma=\frac{1}{\rho_d^0(0)}V^4\frac{1}{\pi}\,\text{Im}\{[G_{d+}^0(0)]^3[NF_0'(0)+F_0(0)^2]\}. \quad \text{(A8)}$$

Let us perform a rough order-of-magnitude estimate of γ. If we assume the impurity level is near the Fermi surface, $G_{d+}^0(0)\cong-i\pi\rho_d^0(0)$ with a vanishing real part. Since $0[|NF_0'(0)|]\sim0[|F_0(0)^2|]\cong N^2/\epsilon_F^2$, and $\rho_d^0(0)\approx1/\Delta_0\cong\epsilon_F/V^2N$, we obtain $\gamma\cong0(1)$.

If the impurity concentration x is not low, Eq. (A7) is not a good approximation and we have to handle Eq. (A1) as we did in Sec. IV.

Calculation of δ

From Eq. (5.28), with the simplification of the type used in Eq. (6.1), we obtain

$$\begin{aligned}\rho_{c2}(0)&=\rho_c^0(0)-x[NV^2(\langle\langle\rho_dI_c^{0''}\rangle\rangle+\langle\langle I_d^0\rho_c^{0''}\rangle\rangle)\\&\qquad+NV^4I_c^{0'}(0)(\langle\langle I_c^{0'}\rho_d'\rangle\rangle+\langle\langle\rho_c^{0'}I_d'\rangle\rangle)]\\&=\rho_c^0(0)(1+\delta x), \quad \text{(A9)}\end{aligned}$$

with

$$\delta\cong-[1/\rho_c^0(0)]NV^2(\langle\langle\rho_d^0I_c^{0''}\rangle\rangle+\langle\langle I_d^0\rho_c^{0''}\rangle\rangle). \quad \text{(A10)}$$

In Eq. (A10), we neglected the higher-order terms in V.

A rough order-of-magnitude estimate of δ can be done as we did for γ. For instance, if we assume the first term in the bracket of Eq. (A10) is dominant and the width of the localized state Δ_0 is smaller than the bandwidth of the host-metal conduction electrons or ϵ_F, the magnitude of γ is estimated to be $\approx0(\Delta_0/\epsilon_F)$.

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[43] For some references, see P. W. Anderson, in *Many-Body Physics*, edited by C. DeWitt and R. Balian (Gordon and Breach, New York, 1968), p. 229.

[44] H. Suhl, Phys. Rev. Letters **19**, 442 (1967); M. Levine and H. Suhl, Phys. Rev. **171**, 567 (1968).