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Strong Correlations in Disordered Systems*

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The effects of strong correlations in a substitutional binary alloy A_xB_{1-x} having a single nondegenerate tight-binding band are examined by use of the coherent-potential approximation and the alloy analogy of Hubbard to treat the effects of disorder and Coulomb interactions, respectively. It is shown that there are no ferromagnetic instabilities in the B band for any band structure, carrier number and the concentration of B atoms, if the potential at A atomic sites are assumed to be positive infinite. This assumption causes the A sites to be inaccessible to electrons. Moreover, the spin susceptibility is found to remain finite even if the density of states is vanishing at the Fermi energy in the limit of the half-filled B band.

I. INTRODUCTION

Since the coherent-potential approximation (CPA)[1,2] was proposed, much progress has been made in the theory of alloys based on a one-electron Hamiltonian. Many-body effects, however, have not yet been discussed extensively. Recently, some authors[3-6] examined the itinerant-electron magnetism of a binary alloy of the type A_xB_{1-x} represented by the Hamiltonian

$$\mathcal{H} = \sum_{i,j,\sigma} t_{ij} a^{\dagger}_{i,\sigma} a_{j,\sigma} + \sum_{i,\sigma} \epsilon^0_i n_{i,\sigma} + \sum_i U_i n_{i,\sigma} n_{i,-\sigma} , \tag{1.1}$$

where $a_{i,\sigma}(a^{\dagger}_{i,\sigma})$ is the annihilation (creation) operator of an electron with spin σ at the ith Wannier site. ϵ^0_i and U_i are assumed to take on values ϵ^0_A, ϵ^0_B and U_A, U_B, respectively.

Hasegawa and Kanamori[3] and Levin *et al.*[4] treated the last term in Eq. (1.1) in the *local* Hartree approximation by writing the atomic energy in the form

$$\epsilon_{i,\sigma} = \epsilon^0_i + U_i \langle n_{i,-\sigma} \rangle . \tag{1.2}$$

In Eq. (1.2), $\langle n_{i,-\sigma} \rangle$ is the average electron number with spin σ at the ith site, which is to be determined self-consistently. They applied the CPA to $\epsilon_{i,\sigma}$. Reference 6 uses this scheme to discuss the dynamical spin susceptibility.

Equation (1.2) is reasonable when the Coulomb interactions are moderately weak. However, as is known, there exist real systems in which the Coulomb forces and therefore the electron correlations are strong. The case of impurity-band conduction in weakly doped uncompensated semiconductors[7] and the alloy of transition-metal oxides[8] are examples. The latter were treated recently by Rice and Brinkman.[9]

The present understanding of the effects of strong correlations is not yet satisfactory even in pure systems. However, the investigations by Hubbard[10] have yielded valuable qualitative insight into this problem. He argues that, if the correlations are sufficiently strong, the quasiparticle energy spectrum has a gap corresponding to the double occupancy of the same site. He identified this gap with the onset of the Mott transition. This type of gap is also expected in alloy systems. Thus two different kinds of gaps will exist in alloys which arise, respectively, from disorder and correlations.

As was shown in Ref. 2, one of the essential parts of Hubbard's approximations, the so-called "scattering correction" in his terminology, is equivalent to the CPA. At a fixed instant in time, the electrons with opposite spins are regarded as

occupying given positions on randomly distributed lattice sites. The configuration average in the alloy problem is here replaced by a time average which arises because these spins are undergoing rearrangements continuously. The approximation which only takes this process into account is called the alloy analogy. In addition to the "scattering correction," he also examined the "resonance-broadening" process arising from the recoil of opposite-spin electrons. By taking these processes into account, he defined the effective atomic energy in the presence of the Coulomb repulsive force in a self-consistent way. This approach of defining effective atomic energies is also applicable to the alloy systems.

The aims of the present investigations are to treat strong correlations in a binary alloy within the framework of the CPA and the Hubbard approximation. We employ the alloy analogy exclusively (except in Sec. IV B) by neglecting the dynamical character of the problem. Although the magnetic properties of *pure systems* have recently been examined,[11] we will add in Sec. II some general results in the present scheme on the spin susceptibility which show that there is no ferromagnetic instability for any single-band model and carrier number except possibly in the case of a precisely half-filled band. The present approach is not applicable to this case if the bands split.

Section III present the general formalism for alloys. Detailed calculations for a somewhat artificial model of an amorphous metal corresponding to the case in which electrons are excluded from A sites are presented in Sec. IV. The conclusions of the present study are summarized in Sec. V.

II. SPIN SUSCEPTIBILITY OF A PURE SYSTEM IN ALLOY ANALOGY

A. Implications of Alloy Analogy

In order to understand the implications of the alloy analogy, we consider, in this section, a pure system by setting $\epsilon_A^0 = \epsilon_B^0 = 0$ and $U_A = U_B = U$ in Eq. (1.1). In the alloy analogy, the original two-body interactions represented by the last term in Eq. (1.1) are approximated by a one-electron energy-dependent potential or effective atomic energy. With the present choice of energy origin, this effective atomic energy E_σ is explicitly given by[2,10]

$$E_\sigma = Un_{-\sigma}[1-(U-E_\sigma)G_\sigma]^{-1}\,, \tag{2.1}$$

where $n_{-\sigma} = \langle n_{i,-\sigma}\rangle$ is the number density per a site of electrons with σ spin and G_σ is the site-diagonal component of the Green's function given by

$$G_\sigma = N^{-1}\sum_k [\epsilon - \epsilon(k) - E_\sigma]^{-1}\,. \tag{2.2}$$

In this equation, N is the total number of lattice sites and $\epsilon(k)$ is defined by

$$\epsilon(k) = \sum_j e^{ik(R_i - R_j)} t_{ij}\,. \tag{2.3}$$

Once $\epsilon(k)$ is explicitly given, the self-consistent equations (2.1) and (2.2) determine G_σ as a function of energy ϵ. In a magnetic field H, n_σ is given in terms of G_σ and the Fermi energy ϵ_F by

$$n_\sigma(H) = -\pi^{-1}\,\mathrm{Im}\int_{-\infty}^{\epsilon_F} d\epsilon\, G_\sigma(\epsilon - \mu_B\sigma H, n_{-\sigma}(H))\,.$$

In this case the paramagnetic spin susceptibility corresponding to uniform magnetic fields can be written

$$\chi = \mu_B\left(\frac{\partial(n_\uparrow - n_\downarrow)}{\partial H}\right)_{H=0} = 2\mu_B\left(\frac{\partial n_\uparrow}{\partial H}\right)_{H=0}.$$

Since

$$\frac{\partial n_\sigma}{\partial H} = -\pi^{-1}\sigma H\,\mathrm{Im}G_\sigma(\epsilon_F, \eta_{-\sigma}(0)) - \pi^{-1}\,\mathrm{Im}\int_{-\infty}^{\epsilon_F} d\epsilon \frac{\partial G_\sigma}{\partial n_{-\sigma}}\frac{\partial n_{-\sigma}}{\partial H}\,,$$

we obtain

$$\chi = 2\mu_B^2\rho[1+K]^{-1}\,, \tag{2.4}$$

where μ_B is the Bohr magneton,

$$\rho = -\pi^{-1}\,\mathrm{Im}G_\sigma(\epsilon_F) \tag{2.5}$$

is the density of states, and

$$K = \frac{\partial n_\sigma}{\partial n_{-\sigma}} \equiv -\pi^{-1}\,\mathrm{Im}\int_{-\infty}^{\epsilon_F} d\epsilon\,\frac{\partial G_\sigma}{\partial n_{-\sigma}}\,. \tag{2.6}$$

It is possible to obtain a band-structure-independent analytic expression for K after some manipulation, which we now outline. The result obtained will be used to show that $\rho(1+K)^{-1}$ in Eq. (2.4) is always positive and finite. Consequently, within the present scheme, the system can never be ferromagnetic.

From the definition [Eq. (2.2)], we have

$$\frac{\partial G_\sigma}{\partial n_{-\sigma}} = S\frac{\partial E_\sigma}{\partial n_{-\sigma}} = S\left[\left(\frac{\partial E_\sigma}{\partial n_{-\sigma}}\right)_{G_\sigma} + \left(\frac{\partial E_\sigma}{\partial G_\sigma}\right)_{n_{-\sigma}}\frac{\partial G_\sigma}{\partial n_{-\sigma}}\right], \tag{2.7}$$

where

$$S = N^{-1}\sum_k [\epsilon - \epsilon(k) - E_\sigma]^{-2}\,. \tag{2.8}$$

Thus,

$$\frac{\partial G_\sigma}{\partial n_{-\sigma}} = S\left[1 - S\left(\frac{\partial E_\sigma}{\partial G_\sigma}\right)_{n_{-\sigma}}\right]^{-1}\left(\frac{\partial E_\sigma}{\partial n_{-\sigma}}\right)_{G_\sigma}. \tag{2.9}$$

On the other hand, Eq. (2.2) also yields

$$\frac{dG_\sigma}{d\epsilon} = -S\left(1 - \frac{dE_\sigma}{d\epsilon}\right) \tag{2.10}$$

$$= -s\left[1-\left(\frac{\partial E_\sigma}{\partial G_\sigma}\right)_{n_{-\sigma}}\frac{dG_\sigma}{d\epsilon}\right]$$

$$= -s\left[1-s\left(\frac{\partial E_\sigma}{\partial G_\sigma}\right)_{n_{-\sigma}}\right]^{-1} . \qquad (2.11)$$

Substituting Eq. (2.9) into (2.6) and eliminating s via (2.11), we get

$$K = \pi^{-1}\,\mathrm{Im}\int_{-\infty}^{\epsilon_F} d\epsilon\,\frac{dG_\sigma}{d\epsilon}\left(\frac{\partial E_\sigma}{\partial n_{-\sigma}}\right)_{G_\sigma}$$

$$= \pi^{-1}\,\mathrm{Im}\int_{G_0}^{G_F} dG_\sigma\left(\frac{\partial E_\sigma}{\partial n_{-\sigma}}\right)_{G_\sigma} , \qquad (2.12)$$

where G_F and G_0 are $G_\sigma(\epsilon=\epsilon_F)$ and $G_\sigma(\epsilon=-\infty)$. In order to evaluate Eq. (2.12) we first transform Eq. (2.1) by introducing $\mathfrak{L}=E_\sigma/U$ and $z=UG_\sigma$, respectively,

$$z\mathfrak{L}^2+(1-z)\mathfrak{L}-n_{-\sigma}=0 \qquad (2.13)$$

or

$$z=(n_{-\sigma}-\mathfrak{L})/(\mathfrak{L}^2-\mathfrak{L}) . \qquad (2.14)$$

In order to express K explicitly in terms of $\mathfrak{L}$, we use Eq. (2.13) and (2.14) to write

$$\left(\frac{\partial E_\sigma}{\partial n_{-\sigma}}\right)_{G_\sigma} = U\left(\frac{\partial \mathfrak{L}}{\partial n_{-\sigma}}\right)_z = U[1+z(2\mathfrak{L}-1)]^{-1}$$

$$= -U[\mathfrak{L}^2+n_{-\sigma}(1-2\mathfrak{L})]^{-1}(\mathfrak{L}^2-\mathfrak{L}) . \qquad (2.15)$$

In addition, from Eq. (2.14), we obtain

$$dG_\sigma = U^{-1}dz = U^{-1}(\mathfrak{L}^2-\mathfrak{L})^{-2}[\mathfrak{L}^2+n_{-\sigma}(1-2\mathfrak{L})]d\mathfrak{L} . \qquad (2.16)$$

Thus,

$$K = -\pi^{-1}\,\mathrm{Im}\int_{\mathfrak{L}_0}^{\mathfrak{L}_F} d\mathfrak{L}\,(\mathfrak{L}^2-\mathfrak{L})^{-1} \qquad (2.17)$$

$$= \pi^{-1}\,\mathrm{Im}\ln[\mathfrak{L}_F(1-\mathfrak{L}_F)^{-1}] , \qquad (2.18)$$

where $\mathfrak{L}_F=\mathfrak{L}(\epsilon=\epsilon_F)$ and $\mathfrak{L}_0=\mathfrak{L}(\epsilon=-\infty)$. The correct branch is obtained by considering $\mathfrak{L}_0=n_{-\sigma}$.

Equation (2.18) is the desired result whose physical implications are discussed below. It is to be emphasized that Eq. (2.18) is valid for any single band $\epsilon(k)$ defined by Eq. (2.3).

We now show that $1+K\geq 0$. Equation (2.14) yields

$$z'' = [\mathfrak{L}'^2+\mathfrak{L}''^2]^{-1}[(\mathfrak{L}'-1)^2+\mathfrak{L}''^2]^{-1}$$

$$\times[\mathfrak{L}''^2+\mathfrak{L}'^2-2n_{-\sigma}\mathfrak{L}'+n_{-\sigma}]\mathfrak{L}'' , \qquad (2.19)$$

where $\mathfrak{L}'$ and $\mathfrak{L}''$ are the real and imaginary parts of $\mathfrak{L}=\mathfrak{L}'+i\mathfrak{L}''$ and similarly for z' and z''. In Eq. (2.19) the first three factors are positive. Furthermore, $z''=UG''\propto -U\rho$ is negative. Thus $\mathfrak{L}''$ is always negative. In addition $\mathrm{Im}\,\mathfrak{L}(1-\mathfrak{L})^{-1}$ appearing in Eq. (2.18) has the same sign as $\mathfrak{L}''$ and is also negative. Consequently, $\mathrm{Im}\ln\mathfrak{L}(1-\mathfrak{L})^{-1}$ can never exceed $-\pi$ for any $\mathfrak{L}$. As a result

$$1+K\geq 0 \qquad (2.20)$$

for any band structure $\epsilon(k)$ and any carrier number $n_{-\sigma}$.

The equality in Eq. (2.20) obtains only for the case where $\mathfrak{L}''=0$ or $\rho(\epsilon_F)=0$ for a half-filled band ($n_\sigma=\frac{1}{2}$), when U is sufficiently large to produce band splitting. Since χ is not determined uniquely for a precisely half-filled band in this case, we consider the spin susceptibility in the limit $n_\sigma\to\frac{1}{2}$. Under these conditions the state density ρ[Eq. (2.5)] is finite and tends to zero. More explicitly,

$$\lim_{n_0\to 1/2}\chi = 2\mu_B^2[\mathfrak{L}_F^2-\mathfrak{L}_F+\tfrac{1}{2}][U\mathfrak{L}_F(\mathfrak{L}_F-1)]^{-1} , \qquad (2.21)$$

which is finite, the factor ρ in Eq. (2.4) having cancelled out. $\mathfrak{L}_F$ is the value of $\mathfrak{L}$ corresponding to the energy at the top of the lower band. Thus we see that spin susceptibility generally remains finite even if the density of states is vanishing at the Fermi energy in the limit of a half-filled band. If we let U in Eq. (2.4) approach infinity,

$$\lim_{U\to\infty}\lim_{n_0\to 1/2}\chi = -\mu_B^2 G_F ,$$

where $G_F=G_\sigma(\epsilon=\epsilon_F)$, which has finite value dependent on the band structure.

Since the dynamical effects of opposite-spin electrons in many cases will reduce the effects of correlations, they will be unfavorable to ferromagnetism. Thus their inclusion would make the possibility of a ferromagnetic instability even less likely. On the basis of this physical argument, one would then conclude that there exists no such instability in the Hubbard model without orbital degeneracy. A more general conjecture of this nature was already made by Van Vleck.[12]

Our arguments apply to the case where there is macroscopic, but possibly infinitesimal, difference of numbers between electrons and the lattice site. In this respect, our statements are not in contradiction with the results of Nagaoka[13] and Thouless,[14] who showed the ground state is ferromagnetic in some lattice structures when U is infinite and the number of electrons Ne satisfies $N-Ne=1$. The case of $Ne=N$, or precisely half-filled band, is very singular. In fact, the electron spins align antiferromagnetically when U is large due to kinetic exchange effects. The Néel temperature T_N is roughly V_0^2/U and as a result χ is divergent as $U\to\infty$. This feature is clearly exhibited by Takahashi[15] for the one-dimensional Hubbard model by use of exact solutions due to Lieb and Wu.[16]

Our present conclusion is also not in disagree-

ment with recent work by Izuyama.[17] He showed that the stiffness constant of spin waves is vanishing by considering the hypothetical case in which all of the electron spins align in one direction in the ground state. This may be taken to imply that the assumed state does not correspond to the spin configuration of the lowest energy.

On the other hand, the spin susceptibility derived by Hubbard's first approximation[18] results in ferromagnetic instabilities.[19] This approximation neglects the self-consistency of Eqs. (2.1) and (2.2) and corresponds to taking $G_\sigma = E^{-1}$ and $E_\sigma = n_{-\sigma}U$ on the right-hand side of Eq. (2.1).

B. Limitations of Alloy Analogy

So far we have treated the correlations among opposite-spin electrons within the alloy analogy. The remaining effects are due to the dynamical nature of the two-body interactions. Although Hubbard has given an approximate treatment of these, their total effects are not yet fully understood. Besides some complicated properties of the problem occurring in the case of $n = \frac{1}{2}$, which we do not treat here, we discuss some of the deficiencies in the present approximation. First, the existence of finite damping of the electrons at the Fermi surface even in pure systems is not consistent with the Fermi liquid theory. This problem was considered by Brinkman and Rice[20] who employed Gutzwiller's variational method[21] to examine the Mott transition in this scheme. This deficiency, however, may not be essential in disordered systems.

Another problem lies in the case of small carrier concentration which has been discussed most rigorously by Kanamori.[22] Within the alloy analogy,

$$E_\sigma = Un_{-\sigma}[1 - UG_\sigma]^{-1}$$

according to Eq. (2.1). By contrast, Kanamori's theory, in which spins $\sigma - \sigma$ are treated on a completely equivalent footing, yields

$$E_\sigma = Un_{-\sigma}[1 - \tfrac{1}{2}UG_\sigma]^{-1} .$$

III. FORMALISM FOR ALLOYS

In the alloy analogy, the effective atomic energy $E_{i\sigma}$ at the ith site is given by

$$E_{i,\sigma} = \epsilon_i^0 + \Delta\epsilon_{i,\sigma} , \tag{3.1}$$

where

$$\Delta\epsilon_{i,\sigma} = U_i \langle n_{i,-\sigma}\rangle [1 - (U_i - \Delta\epsilon_{i,\sigma}) G_{ii,\sigma}]^{-1} \tag{3.2}$$

and ϵ_i^0 and U_i take values ϵ_A^0, ϵ_B^0 and U_A, U_B at A and B sites, respectively. Also the local occupation number is

$$\langle n_{i,\sigma}\rangle = -\pi^{-1} \operatorname{Im} \int_{-\infty}^{\epsilon_F} d\epsilon\, G_{ii,\sigma} , \tag{3.3}$$

where ϵ_F is the Fermi energy. In Eqs. (3.2) and (3.3), $G_{ii,\sigma}$, defined explicitly in Eq. (3.10), is the site-diagonal component of the configuration-averaged Green's function to be determined self-consistently under the constraint that the ith site is occupied by either an A or B atom. The CPA aspects of the problem are described by

$$G_\sigma(k, \epsilon) = [\epsilon - \epsilon(k) - E_{B,\sigma} - \Sigma_\sigma(\epsilon)]^{-1} , \tag{3.4}$$

$$\Sigma_\sigma = \delta_\sigma x[1 - (\delta_\sigma - \Sigma_\sigma)F_\sigma]^{-1} , \tag{3.5}$$

$$\delta_\sigma = E_{A,\sigma} - E_{B,\sigma} , \tag{3.6}$$

$$F_\sigma = \frac{1}{N}\sum_k G_\sigma(k, \epsilon) , \tag{3.7}$$

and

$$\epsilon(k) = \sum_j t_{ij} e^{ik(R_i - R_j)} . \tag{3.8}$$

N is the total number of lattice sites. The local Green's function $G_{ii,\sigma}$ in Eqs. (3.2) and (3.3) is related to F_σ appearing in the preceding equations by

$$G_{ii,\sigma} = F_\sigma[1 - (E_{i,\sigma} - \Sigma_\sigma - E_{B,\sigma})F_\sigma]^{-1} . \tag{3.9}$$

Equations (3.2)–(3.10) must be solved simultaneously. The Fermi energy is determined from the relation

$$\langle n_\sigma\rangle = x\langle n_{A,\sigma}\rangle + y\langle n_{B,\sigma}\rangle = -\pi^{-1} \operatorname{Im} \int_{-\infty}^{\epsilon_F} d\epsilon\, F_\sigma(\epsilon) . \tag{3.10}$$

For appropriate choices of parameters ϵ_i^0, U_i, x, and the band structure $\epsilon(k)$, the present model Hamiltonian Eq. (1.1) can be regarded as providing qualitative insight into the behavior of various systems of physical interest. Typical cases are (i) amorphous transition metals like Ni_4P, Co_4P ($\epsilon_A^0 \to \infty$)[23] and (ii) impurity-band conduction.[7]

The first of these will be examined in Sec. IV.

IV. AMORPHOUS METALS

The one-body Hamiltonian $\mathcal{H}_1$ for a system with vacancies is given by

$$\mathcal{H}_1 = p^2/2m + \sum_l V(r - R_l) , \tag{4.1}$$

where $V(r)$ is the potential due to the ions. Under these circumstances R_l in Eq. (4.1) does not include vacant sites which will be regarded as A atoms. We write Eq. (4.1) as follows:

$$\mathcal{H}_1 = p^2/2m + \sum_n V(r - R_n) - \sum_s V(r - R_s) , \tag{4.2}$$

where R_n runs over all sites, whereas R_s runs over vacant sites only. In the tight-binding approximation, Eq. (4.2) is given by

$$\mathcal{H}_1 = \sum_{i,j} (\epsilon^0 a_i^\dagger a_i + t_{ij} a_i^\dagger a_j) + v\sum_s a_s^\dagger a_s - \sum_{i,s} (t_{is} a_i^\dagger a_s + \text{H.c.}) , \tag{4.3}$$

where i, j run over all sites and s runs over vacant sites alone. In Eq. (4.3), ϵ^0 and v are defined by

$$[p^2/2m + V(r)]\phi(r) = \epsilon_0\phi(r) \ ,$$
$$v \equiv -\int dr\, \phi^*(r) V(r) \phi(r) \ , \tag{4.4}$$

in terms of atomic orbitals $\phi(r)$. On the basis of the virial theorem, $v \cong -2\epsilon^0$. Thus, if $|\epsilon^0|$ is large enough compared with the bandwidth, which is often the case for d bands in real transition metals, we can define the energy origin $\epsilon^0 = 0$ and put $v = \infty$ when there are vacancies present. In this model, each of the vacancies which are randomly distributed in space has the volume of a unit cell. Thus, the atomic density per unit volume is less than that in a perfect crystal. For example, the density of the Bernal structure is 86% of that for the ideal close-packed structure. It must be noted, however, that in a real amorphous material the vacant space is distributed more or less uniformly over the entire solid rather than being confined to lattice sites.

Because the transfer energy between host and impurity sites does not enter the physical result in the case of large atomic energy differences, the model we examine is the same as that of Eq. (1.1) for infinite ϵ_A^0. This limiting case is also applicable to impurity conduction if the main and the impurity bands are well separated.

We consider the paramagnetic state, suppressing the spin suffix, and taking the energy origin as $\epsilon_B^0 = 0$. Moreover, in order to compare the present theoretical results with those of Kimball and Schrieffer,[24] we assume the same density of states function

$$\rho_0(\epsilon) \equiv \frac{1}{N}\sum_k \delta(\epsilon - \epsilon(k)) = \frac{1}{\pi V_0}\left[1 - \left(\frac{\epsilon}{V_0}\right)^2\right]^{-1/2} , \tag{4.5}$$

where V_0 is half of the bandwidth. They represented the interaction energy in the Hamiltonian as

$$U n_{i,\sigma} n_{i,-\sigma} = \tfrac{1}{4}U[(n_{i,\sigma} + n_{i,-\sigma})^2 - (n_{i,\sigma} - n_{i,-\sigma})^2]$$

and calculated the magnetic properties by confining their attention to the second term. Cyrot[25] has examined this problem from the same point of view. For this density of states, Eq. (3.7) can be written

$$FV_0 = (z^2 - 1)^{-1/2} \ , \tag{4.6}$$

where

$$z = (E - E_B - \Sigma)/V_0 \ . \tag{4.7}$$

Since in the limit $\epsilon_A^0 \to \infty$,

$$\Sigma = -x/F, \tag{4.8}$$

Eq. (4.6) can be transformed as

$$\epsilon = E_B - x/F + [V_0^2 + F^{-2}]^{1/2} \ . \tag{4.9}$$

In Eq. (4.9), the branch of square root is the one that gives a positive imaginary part. E_B and $\langle n_{B,\sigma}\rangle$ defined by Eqs. (3.2) and (3.3) can be written

$$E_B = U_B\langle n_B\rangle[1 - (U_B - E_B)F/y]^{-1} \ , \tag{4.10}$$

$$\langle n_B\rangle = -(\pi y)^{-1}\,\mathrm{Im}\int_{-\infty}^{\epsilon_F} d\epsilon\, F \ . \tag{4.11}$$

Equations (4.9) and (4.10) determine F as a function of ϵ with parameters $\langle n_B\rangle$, U_B, and x. Using the F thus obtained, we evaluate the right-hand side of Eq. (4.11) and determine ϵ_F self-consistently.

In Fig. 1, we show the density of states at the Fermi energy

$$\rho = -(1/\pi)\,\mathrm{Im}\,F(\epsilon_F) \tag{4.12}$$

for various values of U_B. y is fixed as $y = 0.8$. As is seen, the B band, which is separated from the A band by disorder, splits when U_B becomes sufficiently large. The critical value of U_B at which splitting first occurs is given by

$$U_B^{(c)}/V_0 = (2y)^{1/2} \ . \tag{4.13}$$

This value is properly compared with the half-width of the B band, W, which is given by

$$W/V_0 = (1 - x^2)^{1/2}. \tag{4.14}$$

Thus,

$$U_B^{(c)}/W = [2(1+x)^{-1}]^{1/2}, \tag{4.15}$$

which is not strongly dependent on x.

A. Spin Susceptibility

The spin susceptibility per B site is

$$\chi = 2\mu_B^2\rho_B[1 + K_{BB}]^{-1}, \tag{4.16}$$

where ρ is the local density of states at B sites given by $\rho_B = \rho/y$ and

$$K_{BB} = \frac{\partial n_{B,\sigma}}{\partial n_{B,-\sigma}} \ . \tag{4.17}$$

By repeating similar manipulations as in Sec. III [cf., Eqs. (3.4), (3.7), (4.8), and (4.10)], we obtain

$$K_{BB} = \pi^{-1}\,\mathrm{Im}\ln[L_F(1 - L_F)^{-1}] \ ,$$

where L_F is the value of $L = E_B/U_B$ at the Fermi energy. Since $\mathrm{Im}E_B \leqq 0$, $\mathrm{Im}L_F(1 - L_F)^{-1} \leqq 0$. Thus, $(1 + K_{BB}) \geqq 0$ as in Sec. II. Hence we conclude again that there is no instability of a paramagnetic state for any $\epsilon(k)$, carrier number, and concentration y except possibly in the case of a precisely half-filled B band to which the present treatment does not apply.

The limiting value of χ for a split B band as $n_B \to \frac{1}{2}$ is generally given by

$$\lim_{n_B \to 1/2} \chi = 2\mu_B^2(L_F^2 - L_F + \tfrac{1}{2})[U_B L_F(L_F - 1)]^{-1}. \tag{4.19}$$

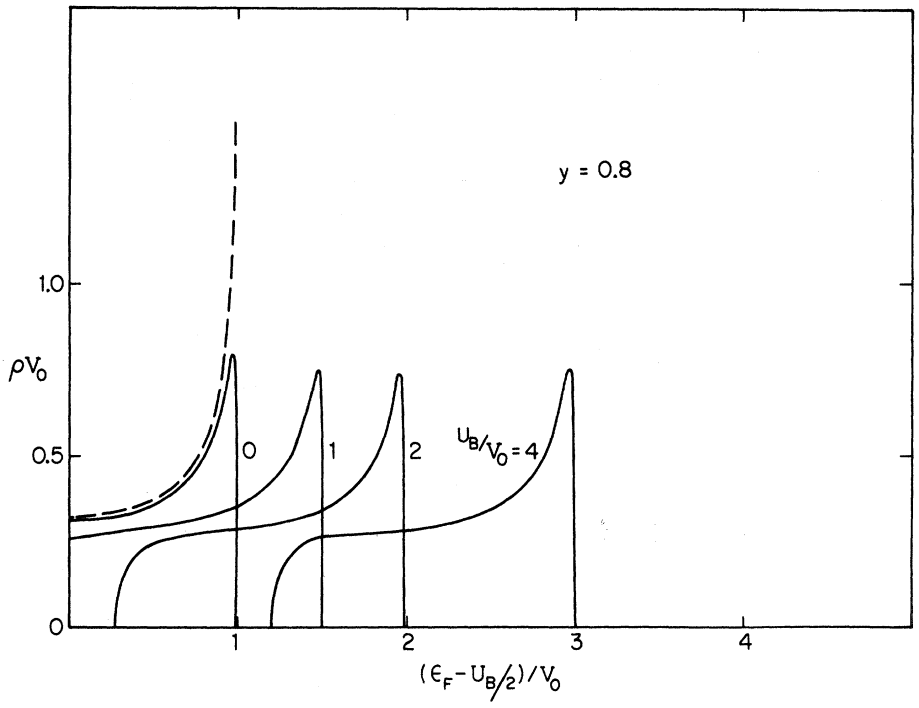

FIG. 1. Density of states at the Fermi energy for various values of U_B for fixed $y = 0.8$. The dashed line corresponds to the perfect crystal with $U_B = 0$. The band splits at the critical value of $U_{B,c}/V_0 = (2y)^{1/2}$.

In the large U_B limit, we have

$$\lim_{U_B\to\infty}\lim_{n_B\to 1/2}\chi = -\mu_B^2 F/y, \tag{4.20}$$

where F is to be evaluated at the upper edge of the lower B band.

For the present state density given by Eq. (4.5), Eq. (4.20) can easily be evaluated using Eq. (4.9) and the fact that $E_B = -n_{-\sigma}y/F$:

$$\lim_{U_B\to\infty}\lim_{n_B\to 1/2}\chi = 2\mu_B^2/V_0(3+x)^{1/2}(1-x)^{-1/2}(1+x)^{-1}. \tag{4.21}$$

In Fig. 2 we show the spin susceptibility per B site in the case of a nearly half-filled B band, i.e.,

$$\lim_{n_B\to 1/2}\chi V_0/2\mu_B^2 \tag{4.22}$$

as a function of U_B/W and for some choice of y. These are depicted by solid lines. U_B is not scaled by V_0 but by W [Eq. (4.14)]. The same quantity in the local Hartree approximation of Eq. (1.2), which results in $K_{BB} = -U_B\rho_B$, is also shown by broken lines. As is explicitly shown, χ is finite and behaves smoothly in the region where the Mott transition sets in. This feature exists for any band structure, $\epsilon(k)$, although we used Eq. (4.5) for explicit evaluation, and is qualitatively in agreement with the observation of Mott[26] in relation to impurity band conduction.

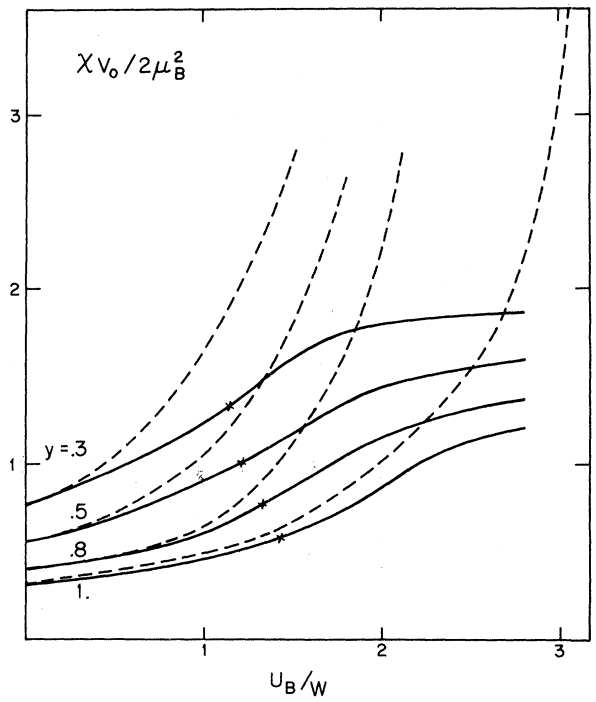

FIG. 2. Paramagnetic spin susceptibility per B lattice site for a nearly half-filled B band [Eq. (4.23)] as a function of U_B/W (solid lines), where W is the B-band halfwidth $(1-x^2)^{1/2}V_0$, which depends on alloy concentration. The susceptibility remains finite, even when the bands have split. · Dashed lines correspond to the Hartree approximation. Bands become split off at the crosses on the solid lines.

B. Degree of the Localization

Confining ourselves to the case of a half-filled B band, we consider the degree of localization de-

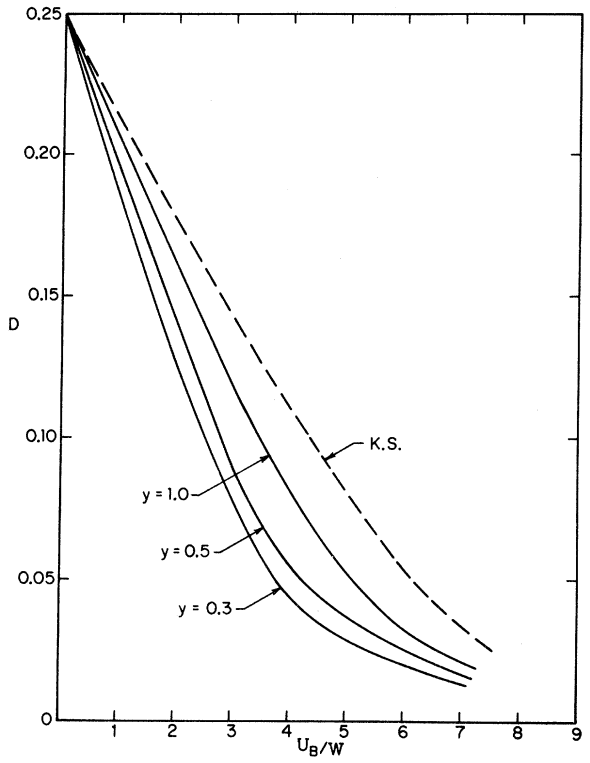

FIG. 3. Degree of localization defined by Eq. (4.24) for various values of y. The "resonance-broadening" effect is included. The result by Kimball and Schreiffer (Ref. 21) is shown by the dashed line.

fined by[24,27]

$$D = (1/Ny) \sum_{i \in B} \langle n_{i,\sigma} n_{i,-\sigma} \rangle . \tag{4.23}$$

If the electrons are itinerant and uncorrelated $D = \frac{1}{4}$, while $D = 0$ when they are completely localized one to each site. Equation (4.23) can be transformed as follows. In the present alloy analogy, the two-body correlation at the ith site is approximated by an energy dependent potential of the electron that occupies this ith site. The decoupling procedure already discussed in connection with Eq. (2.1) may be used to write Eq. (4.23) in the form

$$D = -(\pi y N)^{-1} \sum_{i \in B} \mathrm{Im} \int_{-\infty}^{\epsilon_F} d\epsilon \, G_{ii,\sigma}(\epsilon) \, (E_i / U_i). \tag{4.24}$$

Averaging over possible distributions of B atoms yields

$$D = -\pi^{-1} \mathrm{Im} \int_{-\infty}^{\epsilon_F} d\epsilon \, F[1 + \Sigma F]^{-1} E_B / U_B . \tag{4.25}$$

In the case of $\epsilon_A^0 \to \infty$, Eq. (4.26) becomes

$$D = -(\pi y)^{-1} \mathrm{Im} \int_{-\infty}^{\epsilon_F} d\epsilon \, (E_B / U_B) F. \tag{4.26}$$

It is easy to include the contributions from the "resonance broadening" at this stage. This is useful in the present context in order to permit comparison of the result obtained here with those of Kimball and Schrieffer (KS). Hubbard[10] has shown that the "resonance-broadening" effects are included for a half-filled symmetric band if the scale of U_B is multiplied by 3. Figure 3 shows the degree of localization as a function of U_B/W, where W is the reduced band width associated with the B band. "Resonance-broadening" effects are included as is a comparison with the results obtained by KS. The dashed line denoted by KS is taken from Ref. 24. Compared with KS, the electrons in the present approximation are less mobile. In regard to the concentration dependence, the tendency to localization is seen to be increased as the number of available sites is reduced (y decreasing) even after the scaling of U_B by W. Note that the electrons occupying every B site are completely localized at infinite U_B in the sense

$$\lim_{U_B \to \infty} D = 0.$$

V. CONCLUSION

The present paper has proposed a scheme for treating strong correlations in a binary alloy having a single nondegenerate tight-binding band using the CPA and Hubbard's alloy analogy. It is shown that in the case of a model amorphous metal represented by $\epsilon_A^0 \to \infty$ in the Hamiltonian Eq. (1.1) there are *no* ferromagnetic instabilities in the B band for *any* density-of-states function, carrier number, and concentration of B atoms, y. It should be emphasized that the case of a precisely half-filled split B band is not treated here since the present formalism does not lead to unique results in that case. It is shown in general that the spin susceptibility, χ, per B site in the *nearly* half-filled B band tends to a finite value at large U_B even though the density of states at the Fermi energy is vanishing. Explicit numerical results for χ were obtained in the artificial case of a one-dimensional density of states (Fig. 2). The degree of localization was also examined and is shown in Fig. 3. The tendency to localization is seen to increase with increasing excluded volume.

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Ferromagnetoelastic Resonance in Thin Films. I. Formal Treatment*

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We have undertaken a theoretical study of the effect of magnetoelastic interactions on ferromagnetic resonance in thin films as a possible mechanism for an appreciable anisotropy in resonance linewidth. This study is based on a formalism developed by Tiersten, which is exact within the framework of the quasistatic approximation. The resonance frequency and linewidth are calculated from the simultaneous solution of the coupled magnetoelastic equations of motion under various magnetic and elastic boundary conditions. We find that the magnetoelasticity has an appreciable effect on the resonance linewidth only in the cases where an elastic wave undergoes a thickness resonance near the ferromagnetic-resonance frequency, which we call the "ferromagnetoelastic resonance condition." The above facts have made it possible to develop a self-consistent approximate method, which greatly simplifies the mathematical treatment without sacrificing the physical model. The agreement between the approximate and exact calculations is excellent.

I. INTRODUCTION

The phenomenological Landau–Lifshitz (LL) equation of motion[1] for the magnetization $\vec{M}$, a continuum variable, has been widely used in the study of ferromagnetic resonance (FMR) in thin-metal films.[2–5] The LL equation of motion is applicable to strong ferromagnets, in which the $|\vec{M}|$ can be assumed constant,[6,7] and in which the damping is isotropic.[8]

A similar phenomenological equation of motion can be written for the elastic deformation in the same sample. The two systems of equations can be coupled through a set of quite general magnetoelastic and elastomagnetic coupling terms, as has been shown by Tiersten.[9–11] Approximate solutions have often been obtained by treating the solutions of the uncoupled equations as perturbations upon each other. More realistic solutions are obtained, however, if the coupled sets of equations are solved simultaneously. At a later stage in the development, it becomes possible to treat two sets of polarizations as perturbations upon each other. This simplifies the computations, while retaining the essential features of the coupled system.[12]

In this paper we apply such a method to evaluating the effects of magnetoelasticity on the observed FMR line shape in ferromagnetic-insulator films, using the magnetic parameters corresponding to nickel. A more accurate representation of the nickel-metal film could be obtained by adding an anisotropy field to the LL equation,[12] and by in-