Overhauser[10] dynamic-nuclear-orientation experiment can best be performed when the static field and the time-varying field are applied parallel and perpendicular to the crystal axis, respectively. The best scheme for the Jeffries[11]–Abragam-Proctor[12] effect with noncompeting pumps[13] is ∥ orientation with time-varying field also applied ∥ to crystal axis. The Jeffries–Abragam-Proctor effect with competing pumps[13] can best be obtained when the static and the time-varying fields are applied at angles of 45° and 90°, respectively, with $\phi_1 = 0$ or π.

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Electron Correlation in Ferromagnetism. II. Hybridization of *s* and *d* Bands

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The problem of electron correlation in the ferromagnetism of transition metals is investigated by taking an approximate model Hamiltonian which takes into account the hybridization of the *s* and *d* bands. The Green's-function technique is used to obtain the self-consistent ferromagnetic solutions within the Hartree-Fock approximation. An approximate solution of the correlation problem is obtained. The ferromagnetic solutions for which the correlation effects are taken into account are compared with those in the Hartree-Fock approximation. The model is used to investigate the role of the *s*-*d* interaction in metal-nonmetal transitions. It is also possible to understand the difficulty of observing pressure-induced nonmetal-metal transition.

I. INTRODUCTION

In recent years, much attention has been devoted to the theory of electron correlations in relation to the magnetic properties of transition metals.[1] The electron correlations in the *d* band of transition metals have been studied by Kanamori,[2] Gutzwiller,[3] and Hubbard.[4] These authors based their theories on the assumption that the only interaction responsible for the magnetic properties is the intra-atomic interaction between opposite spin-*d* electrons. Recently, Richmond and Sewell,[5] Pratt and Caron,[6] and Kishore and Joshi[7] took into account the interatomic interaction also. All these investigations completely neglect the presence of the *s* band of conduction electrons.

Anderson's theory[8] of dilute alloys of the transition metals is able to explain the occurrence of the localized magnetic moment on transition-metal impurities dissolved in nonmagnetic metals. In Anderson's model, the band states of the host metal are treated as independent quasiparticles. The impurity is introduced as an extra-localized orbital which is mixed with the band states by a hybrid matrix element. All two-body Coulomb interactions are neglected except the Coulomb interaction between the opposite-spin electrons on the localized orbital. As an extension of this model,

a transition metal can be imagined as a system having a localized d orbital at each lattice site. Recently, such a model has been analyzed by Smith.[9] However, this is an approximate picture of a transition metal, in the sense that there would be no direct interaction between the d electrons on different sites – only an indirect coupling via the conduction electrons. It is well known that a considerable fraction of the width of the $3d$ band in transition metals arises from the overlap of the $3d$ wave functions on neighboring lattice sites.[10]

In this paper, we assume that the d electrons form a band and they interact among themselves only via the Coulomb interaction between opposite-spin electrons at the same lattice site. The effect of the s band is taken into account by adopting the one-particle interaction between s and d electrons given by Anderson. However, for the sake of simplicity we neglect the interatomic Coulomb interaction between d electrons. In Sec. II, we write the Hamiltonian for such a model in the second quantized form. In our analysis, we use the Green's-function method discussed by Zubarev.[11] In Sec. III, the self-consistent ferromagnetic solutions are obtained within the Hartree-Fock approximation for the zero and finite widths of the d band. In Sec. IV, an approximate theory for the electron correlation is developed. The self-consistent ferromagnetic solutions for both the zero and the finite bandwidths of d band are obtained. In Sec. V, the role of the s-d interaction in the metal-nonmetal transition is studied. In Sec. VI, the main results are summarized.

II. BASIC THEORY

We consider a system consisting of s and d electrons described by the Hamiltonian

$$H=\sum_{\vec{k}\sigma} E_{\vec{k}} n_{\vec{k}\sigma}+\sum_{ij\sigma} T_{ij} a^{\dagger}_{i\sigma} a_{j\sigma}+I\sum_{i} n_{i\sigma} n_{i-\sigma} + \sum_{k i\sigma} (V_{\vec{k}d} e^{i\vec{k}\cdot\vec{R}_i} a^{\dagger}_{\vec{k}\sigma} a_{i\sigma} + V^{*}_{\vec{k}d} e^{-i\vec{k}\cdot\vec{R}_i} a^{\dagger}_{i\sigma} a_{\vec{k}\sigma}) , \tag{1}$$

where

$$T_{ij}=\frac{1}{N}\sum_{\vec{k}} (\epsilon_{d\vec{k}}-\mu) e^{i\vec{k}\cdot(\vec{R}_i-\vec{R}_j)} , \qquad E_{\vec{k}}=\epsilon_{\vec{k}}-\mu , \tag{2}$$

$\epsilon_{\vec{k}}$ and $\epsilon_{d\vec{k}}$ are the energies of s- and d-band electrons of wave vector $\vec{k}$, and μ is the Fermi energy. $a^{\dagger}_{\vec{k}\sigma}$, $a_{\vec{k}\sigma}$ are the creation and annihilation operators of the s electron of wave vector $\vec{k}$ and spin σ. $a^{\dagger}_{i\sigma}$, $a_{i\sigma}$ are the same for the d electrons of spin σ at the ith lattice site specified by lattice vector $\vec{R}_i$. I is the Coulomb interaction between electrons of opposite spin at the same lattice site. $n_{\vec{k}\sigma}$ and $n_{i\sigma}$ are, respectively, the number operators for the s electron of wave vector $\vec{k}$ and spin σ, and the d electron of spin σ at the lattice site i. N is the total number of atoms in the system. $V_{\vec{k}d}$ is the hybrid matrix element defined by

$$V_{\vec{k}d}=\int d^3r\, \phi^{*}_{d}(\vec{r}) H_0(\vec{r})\, \psi_{\vec{k}}(\vec{r}) , \tag{3}$$

where $H_0(\vec{r})$ is the one-particle Hamiltonian for an electron in the presence of the periodic lattice, $\phi_d(\vec{r})$ is an atomic d orbital, and $\psi_{\vec{k}}(\vec{r})$ is a Bloch wave function for the conduction band.

The double-time temperature-dependent retarded (+) and advanced (−) Green's functions involving two operators A and B are defined by

$$\langle\langle A(t);\, B(t')\rangle\rangle^{(\pm)} = \mp\, i\,\theta[\pm(t-t')]\,\langle [A(t),\, B(t')]_{\eta}\rangle , \tag{4}$$

where $[A, B]_{\eta}=AB-\eta BA$,

$\eta=\pm$ (whichever is more convenient),

$A(t)=e^{iHt}A(0)e^{-iHt}$.

$\theta(t)$ is the unit step function, unity for positive t and zero for negative t, and $\langle\cdots\rangle$ denotes an average over a grand canonical ensemble at temperature T. We assume $\hbar=1$. In practice, it is convenient to work with the Fourier transform of the Green's function with respect to ω:

$$\langle\langle A; B\rangle\rangle^{(\pm)}_{\omega} = (1/2\pi)\int_{-\infty}^{\infty} \langle\langle A(t);\, B(t')\rangle\rangle^{(\pm)} \times e^{i\omega(t-t')}\, d(t-t') . \tag{5}$$

The Fourier transform satisfies the equation of motion

$$\langle\langle A; B\rangle\rangle_{\omega} = (1/2\pi)\,\langle [A, B]_{\eta}\rangle + \langle\langle [A, H];\, B\rangle\rangle_{\omega} . \tag{6}$$

Here

$$\langle\langle A; B\rangle\rangle_{\omega} = \langle\langle A; B\rangle\rangle^{(+)}_{\omega} \quad \text{if } \mathrm{Im}\omega > 0 \qquad = \langle\langle A; B\rangle\rangle^{(-)}_{\omega} \quad \text{if } \mathrm{Im}\omega < 0, \tag{7}$$

and Im stands for the imaginary part. It can be shown that

$$\langle B(t')A(t)\rangle = i \lim_{\epsilon\to 0^{+}} \int_{-\infty}^{\infty} \frac{\langle\langle A; B\rangle\rangle_{\omega+i\epsilon} - \langle\langle A; B\rangle\rangle_{\omega-i\epsilon}}{(e^{\beta\omega}-\eta)} \times e^{-i\omega(t-t')}\, d\omega , \tag{8}$$

where $\beta=1/k_B T$ and k_B is the Boltzmann constant.

In our analysis we work with Green's functions of the form

$$G^{\sigma}_{\mu\nu}(\omega)=\langle\langle a_{\mu\sigma};\; a^{\dagger}_{\nu\sigma}\rangle\rangle_{\omega} , \quad (\eta=-1) \tag{9}$$

where μ and ν are either the conduction band $\vec{k}$ states or d states on particular lattice sites. Thus we shall have here four different types of Green's functions in all. With the help of the com-

mutators

$$[a_{i\sigma}, H] = \sum_j T_{ij} a_{j\sigma} + In_{i-\sigma} a_{i\sigma} + \sum_{\vec{k}} V^*_{\vec{k}d} e^{-i\vec{k}\cdot\vec{R}_i} a_{\vec{k}\sigma} , \quad (10a)$$

$$[a_{\vec{k}\sigma}, H] = E_{\vec{k}} a_{\vec{k}\sigma} + \sum_i V_{\vec{k}d} e^{i\vec{k}\cdot\vec{R}_i} a_{i\sigma} , \quad (10b)$$

$$[n_{i\sigma}, H] = \sum_j T_{ij}(a^\dagger_{i\sigma} a_{j\sigma} - a^\dagger_{j\sigma} a_{i\sigma}) - \sum_{\vec{k}} V_{\vec{k}d} e^{i\vec{k}\cdot\vec{R}_i} a^\dagger_{\vec{k}\sigma} a_{i\sigma} + \sum_{\vec{k}} V^*_{\vec{k}d} e^{-i\vec{k}\cdot\vec{R}_i} a_{\vec{k}\sigma} a^\dagger_{i\sigma} , \quad (10c)$$

the equations of motion for the Green's functions can be written as

$$(\omega - E_{\vec{k}})\, G^\sigma_{\vec{k}\vec{k}'}(\omega) = \delta_{\vec{k}\vec{k}'}/2\pi + \sum_i V_{\vec{k}d} e^{i\vec{k}\cdot\vec{R}_i} G^\sigma_{i\vec{k}'}(\omega) , \quad (11a)$$

$$(\omega - E_{\vec{k}})\, G^\sigma_{\vec{k}j}(\omega) = \sum_i V_{\vec{k}d} e^{i\vec{k}\cdot\vec{R}_i} G^\sigma_{ij}(\omega) , \quad (11b)$$

$$\omega\, G^\sigma_{ij}(\omega) = \delta_{ij}/2\pi + \sum_l T_{il} G^\sigma_{lj}(\omega) + I\langle\langle n_{i-\sigma} a_{i\sigma}; a^\dagger_{j\sigma}\rangle\rangle_\omega + \sum_{\vec{k}} V^*_{\vec{k}d} e^{-i\vec{k}\cdot\vec{R}_i} G^\sigma_{\vec{k}j}(\omega) , \quad (11c)$$

$$\omega\, G^\sigma_{i\vec{k}'}(\omega) = \sum_j T_{ij} G^\sigma_{j\vec{k}'}(\omega) + I\langle\langle n_{i-\sigma} a_{i\sigma}; a^\dagger_{\vec{k}'\sigma}\rangle\rangle_\omega + \sum_{\vec{k}} V^*_{\vec{k}d} e^{-i\vec{k}\cdot\vec{R}_i} G^\sigma_{\vec{k}\vec{k}'}(\omega) . \quad (11d)$$

We are mainly interested in finding out the Green's functions $G^\sigma_{\vec{k}\vec{k}}(\omega)$ and $G^\sigma_{d\vec{k}}(\omega)$. The latter is defined by

$$G^\sigma_{ij}(\omega) = (1/N)\sum_{\vec{k}} G^\sigma_{d\vec{k}}(\omega)\, e^{i\vec{k}\cdot(\vec{R}_i - \vec{R}_j)} . \quad (12)$$

These Green's functions are needed to evaluate the average number $\langle n_{s\sigma}\rangle$ of s electrons and $\langle n_{d\sigma}\rangle$ of d electrons per atom for spin σ. By taking the limit $t \to t'$ in Eq. (8), we get $\langle n_{s\sigma}\rangle$ and $\langle n_{d\sigma}\rangle$ as

$$\langle n_{s\sigma}\rangle = (1/N)\sum_{\vec{k}} \langle a^\dagger_{\vec{k}\sigma} a_{\vec{k}\sigma}\rangle = \int_{-\infty}^{\infty} \rho^\sigma_s(\omega)\,(e^{\beta\omega}+1)^{-1} d\omega , \quad (13)$$

$$\langle n_{d\sigma}\rangle = (1/N)\sum_i \langle a^\dagger_{i\sigma} a_{i\sigma}\rangle = \int_{-\infty}^{\infty} \rho^\sigma_d(\omega)\,(e^{\beta\omega}+1)^{-1} d\omega , \quad (14)$$

where

$$\rho^\sigma_s(\omega) = \frac{i}{N} \lim_{\epsilon\to 0^+} \sum_{\vec{k}} [G^\sigma_{\vec{k}\vec{k}}(\omega + i\epsilon) - G^\sigma_{\vec{k}\vec{k}}(\omega - i\epsilon)] , \quad (15)$$

$$\rho^\sigma_d(\omega) = \frac{i}{N} \lim_{\epsilon\to 0^+} \sum_{\vec{k}} [G^\sigma_{d\vec{k}}(\omega + i\epsilon) - G^\sigma_{d\vec{k}}(\omega - i\epsilon)] \quad (16)$$

are the desntiy of states per atom for s and d electrons corresponding to spin σ. The total average number of electrons per atom for spin σ is given by

$$\langle n_\sigma\rangle = \langle n_{s\sigma}\rangle + \langle n_{d\sigma}\rangle . \quad (17)$$

III. HARTREE-FOCK THEORY

For the sake of comparison with the results of the theory to be developed in Sec. IV for the correlation effects, it would be useful to investigate the problem in the Hartree-Fock approximation. Actually, we shall not make an exhaustive study of all possible Hartree-Fock solutions, but will restrict ourselves to particularly simple solutions which may represent paramagnetic or ferromagnetic states but not more complicated spin arrangements. The same restriction applies to the scope of the correlation theory developed in Sec. IV.

In terms of the Green's functions, the Hartree-Fock approximation corresponds to the assumption that

$$\langle\langle n_{i-\sigma} a_{i\sigma};\ a^\dagger_{\mu\sigma}\rangle\rangle_\omega \simeq \langle n_{i-\sigma}\rangle \langle\langle a_{i\sigma};\ a^\dagger_{\mu\sigma}\rangle\rangle_\omega , \quad (18)$$

where index μ is either j or $\vec{k}$. We restrict ourselves to the class of solutions for which $\langle n_{i-\sigma}\rangle$ is independent of the lattice site i,

$$\langle n_{i\sigma}\rangle = \langle n_{d\sigma}\rangle \text{ for all } i . \quad (19)$$

When we incorporate the assumptions (18) and (19) in Eqs. (11c) and (11d), Eqs. (11a)–(11d) assume a closed form. Solutions of these equations for $G^\sigma_{\vec{k}\vec{k}}(\omega)$ and $G^\sigma_{d\vec{k}}(\omega)$ give

$$G^\sigma_{\vec{k}\vec{k}}(\omega) = \frac{\omega - E_{d\vec{k}} - I\langle n_{d-\sigma}\rangle}{\omega - E_{\vec{k}}}\, G^\sigma_{d\vec{k}}(\omega) , \quad (20)$$

$$G^\sigma_{d\vec{k}}(\omega) = \frac{1/2\pi}{\omega - E_{d\vec{k}} - I\langle n_{d-\sigma}\rangle - N|V_{\vec{k}d}|^2(\omega - E_{\vec{k}})} . \quad (21)$$

By substituting the values of $G^\sigma_{\vec{k}\vec{k}}(\omega)$ and $G^\sigma_{d\vec{k}}(\omega)$ from Eqs. (20) and (21) in Eqs. (15) and (16), we obtain the density of states per atom of s and d electrons corresponding to spin σ:

$$\rho^\sigma_s(\omega) = (1/N)\sum_{\vec{k}} [A^+_{s\vec{k}\sigma}\delta(\omega - \omega^+_{\vec{k}\sigma}) + A^-_{s\vec{k}\sigma}\delta(\omega - \omega^-_{\vec{k}\sigma})] , \quad (22)$$

$$\rho^\sigma_d(\omega) = (1/N)\sum_{\vec{k}} [A^+_{d\vec{k}\sigma}\delta(\omega - \omega^+_{\vec{k}\sigma}) + A^-_{d\vec{k}\sigma}\delta(\omega - \omega^-_{\vec{k}\sigma})] , \quad (23)$$

where

$$\omega^p_{\vec{k}\sigma} = \tfrac{1}{2}\{E_{\vec{k}} + E_{d\vec{k}} + I\langle n_{d-\sigma}\rangle + p[(E_{d\vec{k}} - E_{\vec{k}} + I\langle n_{d-\sigma}\rangle)^2 + 4N|V_{\vec{k}d}|^2]^{1/2}\} , \quad (24)$$

$$A^p_{s\vec{k}\sigma} = p\,\frac{\omega^p_{\vec{k}\sigma} - E_{d\vec{k}} - I\langle n_{d-\sigma}\rangle}{\omega^+_{\vec{k}\sigma} - \omega^-_{\vec{k}\sigma}} , \quad (25)$$

$$A^p_{d\vec{k}\sigma} = p\,(\omega^p_{\vec{k}\sigma} - E_{\vec{k}})/(\omega^+_{\vec{k}\sigma} - \omega^-_{\vec{k}\sigma}) . \quad (26)$$

Here p is either (+) or (−).

The expressions (22) and (23) for the density of

states per atom of s and d electrons corresponding to spin σ show that s and d bands are admixed into two new bands with dispersion laws $\omega = \omega^{+}_{\vec{k}\sigma}$ and $\omega = \omega^{-}_{\vec{k}\sigma}$. The general form of these bands is shown in Fig. 1. For an unperturbed d band, $\epsilon_{d\vec{k}}$ of zero width, the new bands are always separated by an energy gap. In this core the lower band always lies below $T_0 - \mu + I\langle n_{d-\sigma}\rangle$ while the upper band always lies above this energy. Here T_0 is the mean energy of the d band $\epsilon_{d\vec{k}}$. As the width of the band $\epsilon_{d\vec{k}}$ increases, the gap between the two bands decreases and finally they overlap each other. From Eqs. (25) and (26) it is clear that $A^{-}_{s\vec{k}\sigma} + A^{-}_{d\vec{k}\sigma} = A^{+}_{s\vec{k}\sigma} + A^{+}_{d\vec{k}\sigma} = 1$. This shows that for both the new bands the density of states per atom for each spin is always equal to 1. Therefore, if there are two electrons per atom in the two bands together, then for the zero width of the d bands, the system always behaves as an insulator. As we increase the d-band width, an insulator-to-metal transition occurs at some critical d-band width. In Sec. V, we shall discuss this type of transition in detail for the the case $I = 0$.

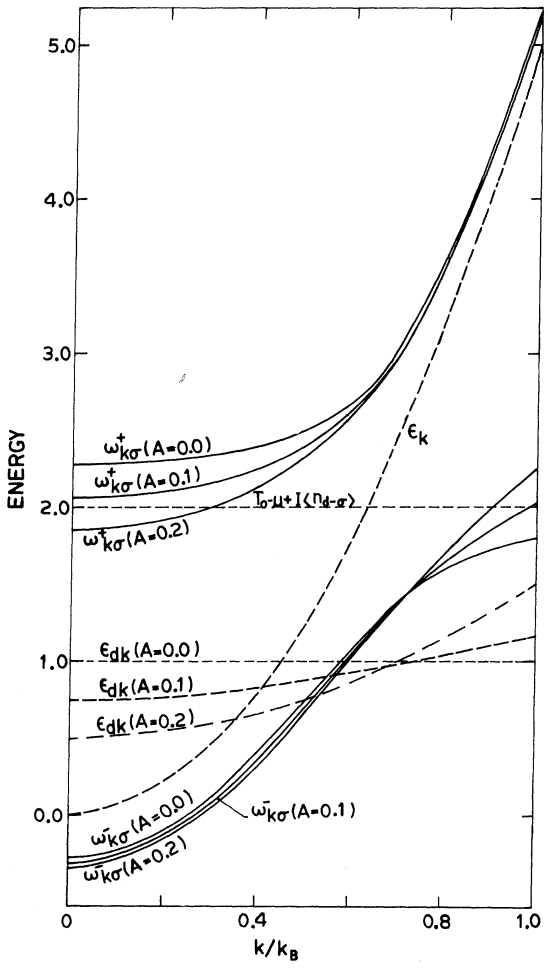

FIG. 1. Hybrid bands in the Hartree-Fock approximation for zero and finite d-band width. The parameters are expressed in terms of T_0. The parameters corresponding to this figure are $T_0 = 1.0$, $I = 2.0$, $v = 0.8$, $\alpha = 5.0$, and $\langle n_{d-\sigma}\rangle = 0.5$. k_B is the wave vector to the zone boundary.

A. Zero Bandwidth

In the limit of the zero bandwidth, $\epsilon_{d\vec{k}} = T_0$ for all $\vec{k}$. It is easy to show from Eq. (24) that

$$\omega^{-}_{\vec{k}\sigma} < E_{\vec{k}} < \omega^{+}_{\vec{k}\sigma}$$

and $$\omega^{-}_{\vec{k}\sigma} < (E_{d\vec{k}} + I\langle n_{d-\sigma}\rangle) < \omega^{+}_{\vec{k}\sigma} ,$$

so that $A^{p}_{s\vec{k}\sigma}$ and $A^{p}_{d\vec{k}\sigma}$ are positive. Then by replacing $\epsilon_{d\vec{k}}$ by T_0 in Eqs. (22) and (23), we get

$$\rho^{\sigma}_{s}(\omega) = (1/N)\textstyle\sum_{\vec{k}} |\omega + \mu - T_0 - I\langle n_{d-\sigma}\rangle| \times \delta[(\omega - \omega^{+}_{\vec{k}\sigma})(\omega - \omega^{-}_{\vec{k}\sigma})] , \quad (27)$$

$$\rho^{\sigma}_{d}(\omega) = (1/N)\textstyle\sum_{\vec{k}} |\omega + \mu - \epsilon_{\vec{k}}| \times \delta[(\omega - \omega^{+}_{\vec{k}\sigma})(\omega - \omega^{-}_{\vec{k}\sigma})] . \quad (28)$$

For the sake of simplicity, we assume that the hybrid matrix element $V_{\vec{k}d}$ is independent of $\vec{k}$. Then these equations can be expressed in terms of the density of states for the s band,

$$N(\omega) = (1/N)\textstyle\sum_{\vec{k}} \delta(\omega - \epsilon_{\vec{k}}) , \quad (29)$$

which is normalized to unity since $\vec{k}$ is limited to the first Brillouin zone and the higher plane-wave bands will be neglected. In terms of $N(\omega)$, Eqs. (28) and (29) can be written as

$$\rho^{\sigma}_{s}(\omega) = N[f_\sigma(\omega + \mu)] , \quad (30)$$

$$\rho^{\sigma}_{d}(\omega) = \left| \frac{\omega + \mu - f_\sigma(\omega + \mu)}{\omega + \mu - T_0 - I\langle n_{d-\sigma}\rangle} \right| N[f_\sigma(\omega + \mu)] , \quad (31)$$

where $$f_\sigma(\omega) = \omega - |v|^2/(\omega - T_0 - I\langle n_{d-\sigma}\rangle) , \quad (32)$$

$$|v|^2 = N|V_{\vec{k}d}|^2 . \quad (33)$$

Finally, the average numbers of s and d electrons per atom for spin σ at absolute zero are given by

$$\langle n_{s\sigma}\rangle = \int_{-\infty}^{\mu} N[f_\sigma(\omega)]\, d\omega \quad (34)$$

and

$$\langle n_{d\sigma}\rangle = \int_{-\infty}^{\mu} \left| \frac{\omega - f_\sigma(\omega)}{\omega - T_0 - I\langle n_{d-\sigma}\rangle} \right| N[f_\sigma(\omega)]\, d\omega . \quad (35)$$

These equations give the total average number of electrons per atom for spin σ at absolute zero.

$$\langle n_\sigma\rangle = \int_{-\infty}^{\mu} \left(1 + \left| \frac{\omega - f_\sigma(\omega)}{\omega - T_0 - I\langle n_{d-\sigma}\rangle} \right|\right) N[f_\sigma(\omega)]\, d\omega . \quad (36)$$

With the Fermi level as a variable parameter, Eq. (35) for $\langle n_{d\sigma}\rangle$ must be solved self-consistently. Then Eq. (36) can be used to fix the Fermi level from the total number of electrons per atom $n = \langle n_+\rangle + \langle n_-\rangle$ which is assumed given. The ferromagnetic solutions are possible only when $\langle n_{d\sigma}\rangle \neq \langle n_{d-\sigma}\rangle$. Solutions of the integrals (35) and (36) depend on the form of the density of states $N(\omega)$. For simplicity, we consider the square density of states defined by

$$N(\omega) = 1/\alpha \quad \text{if } 0 < \omega < \alpha$$
$$= 0 \quad \text{otherwise,} \tag{37}$$

where α is the width of the s band. For the square density of states we have

$$N[f_\sigma(\omega)] = \frac{1}{\alpha}\sum_{p=\pm}[\theta(\omega-\omega_{1\sigma}^p)-\theta(\omega-\omega_{2\sigma}^p)] \ , \tag{38}$$

where

$$\omega_{1\sigma}^p = \tfrac{1}{2}\{T_0 + I\langle n_{d-\sigma}\rangle + p\,[(T_0+I\langle n_{d-\sigma}\rangle)^2 + 4|v|^2]^{1/2}\},$$
$$\omega_{2\sigma}^p = \tfrac{1}{2}\{\alpha + T_0 + I\langle n_{d-\sigma}\rangle + p\,[(T_0+I\langle n_{d-\sigma}\rangle - \alpha)^2 + 4|v|^2]^{1/2}\}.$$

Now we substitute the values of $f_\sigma(\omega)$ and $N[f_\sigma(\omega)]$ from Eqs. (32) and (38) in Eqs. (35) and (36) and get

$$\langle n_{d\sigma}\rangle = \int_{-\infty}^{\mu}(|v|^2\sum_{p=\pm}[\theta(\omega-\omega_{1\sigma}^p)-\theta(\omega-\omega_{2\sigma}^p)]/ \alpha(\omega - T_0 - I\langle n_{d-\sigma}\rangle)^2)\,d\omega \ , \tag{39}$$

$$\langle n_\sigma\rangle = \int_{-\infty}^{\mu}(1/\alpha)\{1+[|v|^2/(\omega - T_0 - I\langle n_{d-\sigma}\rangle)^2]\} \times \sum_{p=\pm}[\theta(\omega-\omega_{1\sigma}^p)-\theta(\omega-\omega_{2\sigma}^p)]d\omega \ . \tag{40}$$

Integrals (39) and (40) are easy to evaluate. The limits of integrations are controlled by the θ functions.

Now by taking μ as a variable parameter we solve Eq. (39) self-consistently for some particular choice of parameters I, α, and T_0 to obtain $\langle n_{d\sigma}\rangle$ and $\langle n_{d-\sigma}\rangle$. Then Eq. (40) is used to fix the value of μ for the integral values ($n = 1, 2, 3$) of the total number of electrons in both the bands together. We do not consider $n = 4$ because in this case both the bands are completely filled and hence there is no possibility of ferromagnetism. In Fig. 2 we have plotted $Q = \mu/T_0$ versus $Z = T_0/\alpha$ for three values 0.1, 0.2, and 1.0 of $S = |v|/T_0$ for a particular value of $P = I/T_0 = 2.0$. The range of existence of the ferromagnetic solutions between the values of Z from 0 to 1 is shown in Table I. The value of Q corresponding to a particular value of Z can be read from Fig. 2. To show explicitly the magnetic solutions, we have plotted $\langle n_{d+}\rangle$ and $\langle n_{d-}\rangle$ in Fig. 3. Results of our calculations show that the range of the ferromagnetic solutions decreases as the hybridization of s and d bands increases, i.e., the hybridization of s and d bands decreases the tendency towards ferromagnetism. To have an idea about the variation of the ferromagnetic solutions with respect to the strength of interatomic interaction, we have plotted Q versus Z in Fig. 4 for three different values of P, 0.5, 1.0, and 2.0 and for a particular value of $S = 0.1$. The range of ferromagnetic solutions is shown in Table II. It is found that the increase of intra-atomic interaction is favorable to ferromagnetism.

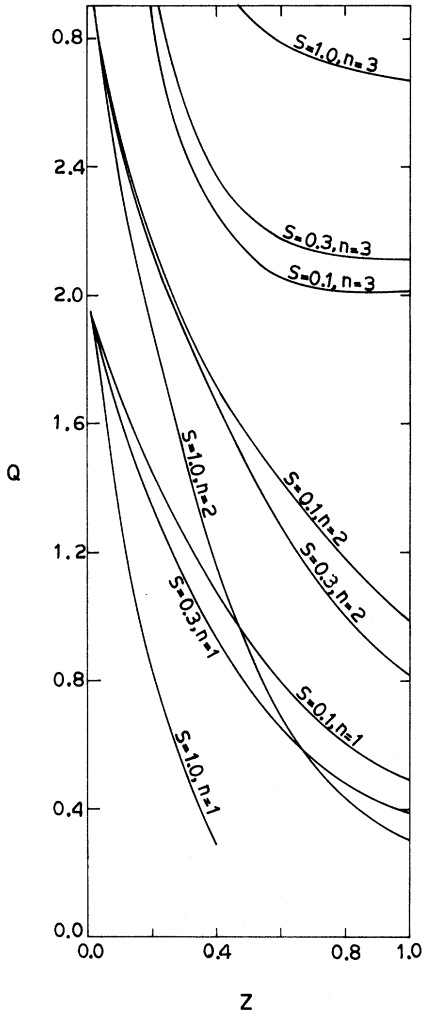

FIG. 2. Variation of Fermi level with Z in the Hartree-Fock approximations for zero width of d band and square density of states for s band. Curves are plotted for $P = 2.0$.

TABLE I. Range of Z for ferromagnetic solutions for zero width of the d band.

P	S	n	Z
2.0	0.1	1.0	0.01–0.45
		2.0	0.05–0.95
		3.0	0.4 –1.0
	0.3	1.0	0.01–0.35
		2.0	0.05–0.65
		3.0	0.2 –1.0
	1.0	1.0	0.01–0.2
		2.0	0.01–0.1
		3.0	0.4 –1.0

B. Finite Bandwidth

We shall assume that the form of the d band is the same as that of the s band. We represent it by the expression

$$\epsilon_{d\vec{k}} = A\epsilon_{\vec{k}} + T_0 - \tfrac{1}{2}A\alpha \ , \tag{41}$$

where A is some positive constant less than unity, i.e., it is assumed that the width of d band is smaller than that of the s band. $A = 0$ corresponds to the zero bandwidth. This choice is made because the density of states $\rho_s^\sigma(\omega)$ and $\rho_d^\sigma(\omega)$ given by Eqs. (22) and (23) can then be expressed in terms of the density of states of the s band, $N(\omega)$. Substituting the expression (41) for $\epsilon_{d\vec{k}}$ in Eqs. (22) and (23) and using the approximation (33), we get

$$\rho_s^\sigma(\omega) = \frac{1}{N}\sum_{\vec{k}} \left| \frac{\omega + \mu - A\epsilon_{\vec{k}} - T_0 + \frac{1}{2}A\alpha - I\langle n_{d-\sigma}\rangle}{A} \right| \times \delta\{[g_\sigma^+(\omega+\mu) - \epsilon_{\vec{k}}][g_\sigma^-(\omega+\mu) - \epsilon_{\vec{k}}]\}, \tag{42}$$

$$\rho_d^\sigma(\omega) = (1/N)\sum_{\vec{k}} [(\omega + \mu - \epsilon_{\vec{k}})/A] \times \delta\{[g_\sigma^+(\omega+\mu) - \epsilon_{\vec{k}}][g_\sigma^-(\omega+\mu) - \epsilon_{\vec{k}}]\}, \tag{43}$$

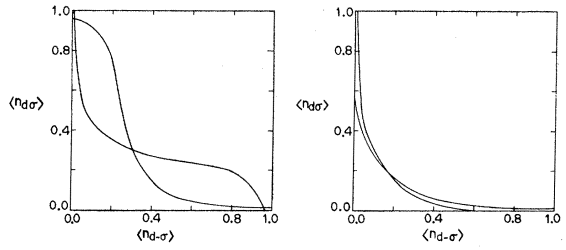

FIG. 3. Self-consistent magnetic solutions in the Hartree-Fock approximations for zero d-band width and the square density of states for the s band. The parameters used are (a) $P = 2.0$, $S = 0.3$, $n = 2.0$, $Z = 0.45$, and $Q = 1.56$; (b) $P = 2.0$, $S = 0.3$, $n = 2.0$, $Z = 0.7$, and $Q = 1.12$.

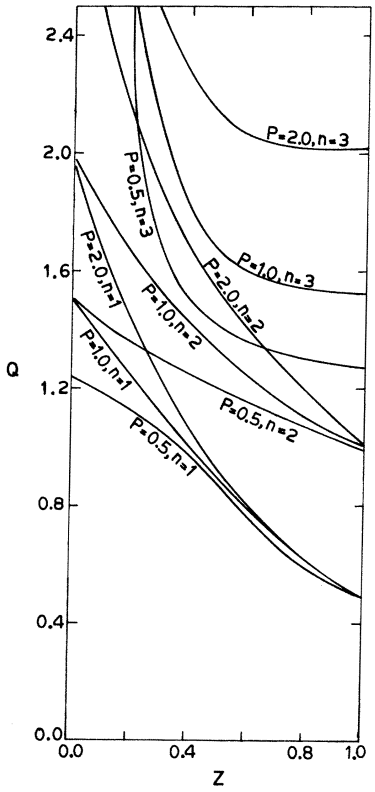

FIG. 4. Variation of the Fermi level with Z in the Hartree-Fock approximation for zero d-band width and the square density of states for s band. Curves are plotted for $S = 0.1$.

where

$$g_\sigma^p(\omega) = (1/2A)\left((A+1)\omega - T_0 + \tfrac{1}{2}A\alpha - I\langle n_{d-\sigma}\rangle + p\{[(1-A)\omega - T_0 + \tfrac{1}{2}A\alpha - I\langle n_{d-\sigma}\rangle]^2 + 4A|v|^2\}^{1/2}\right) . \tag{44}$$

Equations (42) and (43) can be written in terms of the density of states $N(\omega)$:

TABLE II. Range of Z for ferromagnetic solutions for zero width of the d band.

S	P	n	Z
0.1	0.5	1.0	0.01–0.35
		2.0	0.1 –0.85
		3.0	0.4 –1.0
	1.0	1.0	0.01–0.45
		2.0	0.05–0.95
		3.0	0.4 –1.0
	2.0	1.0	0.01–0.45
		2.0	0.05–0.95
		3.0	0.4 –1.0

$$\rho_s^\sigma(\omega)=\frac{1}{A}\sum_{p=\pm}\left|\frac{\omega+\mu-T_0+\frac{1}{2}A\alpha-I\langle n_{d-\sigma}\rangle-Ag_\sigma^p(\omega+\mu)}{g_\sigma^+(\omega+\mu)-g_\sigma^-(\omega+\mu)}\right| \times N[g_\sigma^p(\omega+\mu)], \tag{45}$$

$$\rho_d^\sigma(\omega)=\frac{1}{A}\sum_{p=\pm}\left|\frac{\omega+\mu-g_\sigma^p(\omega+\mu)}{g_\sigma^+(\omega+\mu)-g_\sigma^-(\omega+\mu)}\right| N[g_\sigma^p(\omega+\mu)]. \tag{46}$$

For the square density of states for the unperturbed s band, $N[g_\sigma^p(\omega+\mu)]$ is given by

$$N[g_\sigma^p(\omega+\mu)]=\frac{1}{\alpha}[\theta(\omega+\mu-\omega_{1\sigma}^{-p})-\theta(\omega+\mu-\omega_{2\sigma}^{-p})], \tag{47}$$

where

$$\omega_{1\sigma}^p=\tfrac{1}{2}\{T_0-\tfrac{1}{2}A\alpha+I\langle n_{d-\sigma}\rangle +p[(T_0-\tfrac{1}{2}A\alpha+I\langle n_{d-\sigma}\rangle)^2+4|v|^2]^{1/2}\}, \tag{48}$$

and

$$\omega_{2\sigma}^p=\tfrac{1}{2}((\tfrac{1}{2}A+1)\alpha+T_0+I\langle n_{d-\sigma}\rangle +p\{[(\tfrac{1}{2}A-1)\alpha+T_0+I\langle n_{d-\sigma}\rangle]^2+4|v|^2\}^{1/2}). \tag{49}$$

By substituting the values of $g_\sigma^p(\omega+\mu)$ and $N[g_\sigma^p\times(\omega+\mu)]$ from Eqs. (44) and (47) in Eqs. (45) and (46) we get at absolute zero

$$\langle n_{s\sigma}\rangle=\int_{-\infty}^{\mu}\frac{1}{2\alpha}\sum_{p=\pm}\left(1-p\frac{(1-A)\omega-T_0+\frac{1}{2}A\alpha-I\langle n_{d-\sigma}\rangle}{\{[(1-A)\omega-T_0+\frac{1}{2}A\alpha-I\langle n_{d-\sigma}\rangle]^2+4A|v|^2\}^{1/2}}\right)[\theta(\omega-\omega_{1\sigma}^{-p})-\theta(\omega-\omega_{2\sigma}^{-p})]d\omega, \tag{50}$$

$$\langle n_{d\sigma}\rangle=\frac{1}{2A\alpha}\sum_{p=\pm}\left(1+p\frac{(1-A)\omega-T_0+\frac{1}{2}A\alpha-I\langle n_{d-\sigma}\rangle}{\{[(1-A)\omega-T_0+\frac{1}{2}A\alpha-I\langle n_{d-\sigma}\rangle]^2+4A|v|^2\}^{1/2}}\right)[\theta(\omega-\omega_{1\sigma}^{-p})-\theta(\omega-\omega_{2\sigma}^{-p})]d\omega. \tag{51}$$

As in the case of the zero bandwidth, by taking μ as a variable parameter $\langle n_{d\sigma}\rangle$ and $\langle n_{d-\sigma}\rangle$ are obtained self-consistently from Eq. (51). Then Eqs. (17) and (50) are used to fix the Fermi level for an integral number of electrons. In Fig. 5, Q-versus-Z curves are shown for three values 0.1, 0.2, and 0.4 of A. Values of P and S are taken equal to 2.0 and 0.1, respectively. Table III indicates that the range of the ferromagnetic solutions diminishes as the d-band width increases. This shows that the localization of the d electrons favors the existence of ferromagnetism.

IV. CORRELATION THEORY

In this section we discuss the effect of correlation by considering the equation of motion of the higher-order Green's function $\langle\langle n_{i-\sigma}a_{i\sigma};\ a_{\mu\sigma}^\dagger\rangle\rangle_\omega$, where μ is either j or $\vec{k}'$. The equation of motion for this Green's function is given by

$$\begin{aligned}\omega\langle\langle n_{i-\sigma}a_{i\sigma};\ a_{\mu\sigma}^\dagger\rangle\rangle_\omega &=\frac{\langle n_{i-\sigma}\rangle\delta_{ij\mu}}{2\pi}+\sum_l T_{il}\langle\langle n_{i-\sigma}a_{l\sigma};\ a_{\mu\sigma}^\dagger\rangle\rangle_\omega\\ &+I\langle\langle n_{i-\sigma}a_{i\sigma};\ a_{\mu\sigma}^\dagger\rangle\rangle_\omega\\ &+\sum_{\vec{k}}V_{\vec{k}d}^*e^{-i\vec{k}\cdot\vec{R}_i}\langle\langle n_{i-\sigma}a_{\vec{k}\sigma};\ a_{\mu\sigma}^\dagger\rangle\rangle_\omega\\ &+\sum_l T_{il}\langle\langle(a_{i-\sigma}^\dagger a_{l-\sigma}-a_{l-\sigma}^\dagger a_{i-\sigma})a_{i\sigma};\ a_{\mu\sigma}^\dagger\rangle\rangle_\omega\\ &-\sum_{\vec{k}}V_{\vec{k}d}e^{i\vec{k}\cdot\vec{R}_i}\langle\langle a_{\vec{k}-\sigma}^\dagger a_{i-\sigma}a_{i\sigma};\ a_{\mu\sigma}^\dagger\rangle\rangle_\omega\\ &+\sum_{\vec{k}}V_{\vec{k}d}^*e^{-i\vec{k}\cdot\vec{R}_i}\langle\langle a_{\vec{k}-\sigma}a_{i-\sigma}^\dagger a_{i\sigma};\ a_{\mu\sigma}^\dagger\rangle\rangle_\omega.\end{aligned} \tag{52}$$

We assume that the correlations between electrons at different lattice sites and the correlation between s and d electrons are very small as compared to the correlation between electrons at the same lattice site. In this approximation, we can decouple the Green's functions on the right-hand side of Eq. (52) by replacing the operators at the same lattice site with their average values as follows:

$$\langle\langle n_{i-\sigma}a_{l\sigma};\ a_{\mu\sigma}^\dagger\rangle\rangle_\omega\simeq\langle n_{d-\sigma}\rangle\langle\langle a_{l\sigma};\ a_{\mu\sigma}^\dagger\rangle\rangle_\omega \quad \text{if } i\neq l,$$

$$\langle\langle a_{i-\sigma}^\dagger a_{l-\sigma}a_{i\sigma};\ a_{\mu\sigma}^\dagger\rangle\rangle_\omega \simeq-\langle a_{i-\sigma}^\dagger a_{i\sigma}\rangle\langle\langle a_{l-\sigma};\ a_{\mu\sigma}^\dagger\rangle\rangle_\omega \quad \text{if } i\neq l,$$

$$\langle\langle a_{l-\sigma}^\dagger a_{i-\sigma}a_{i\sigma};\ a_{\mu\sigma}^\dagger\rangle\rangle_\omega \simeq\langle a_{i-\sigma}a_{i\sigma}\rangle\langle\langle a_{l-\sigma}^\dagger;\ a_{\mu\sigma}^\dagger\rangle\rangle_\omega \quad \text{if } i\neq l,$$

$$\langle\langle n_{i-\sigma}a_{k\sigma};\ a_{\mu\sigma}^\dagger\rangle\rangle_\omega\simeq\langle n_{d-\sigma}\rangle\langle\langle a_{k\sigma};\ a_{\mu\sigma}^\dagger\rangle\rangle_\omega,$$

$$\langle\langle a_{\vec{k}-\sigma}^\dagger a_{i-\sigma}a_{i\sigma};\ a_{\mu\sigma}^\dagger\rangle\rangle_\omega$$

$$\simeq \langle a_{i-\sigma} a_{i\sigma}\rangle \langle\langle a^{\dagger}_{\vec{k}-\sigma}; a^{\dagger}_{\mu\sigma}\rangle\rangle_{\omega} ,$$

$$\langle\langle a_{\vec{k}-\sigma} a^{\dagger}_{i-\sigma} a_{i\sigma}; a^{\dagger}_{\mu\sigma}\rangle\rangle_{\omega} \simeq \langle a^{\dagger}_{i-\sigma} a_{i\sigma}\rangle \langle\langle a_{\vec{k}-\sigma}; a^{\dagger}_{\mu\sigma}\rangle\rangle_{\omega} . \quad (53)$$

We also assume that

$$\langle a^{\dagger}_{i-\sigma} a_{i\sigma}\rangle = \langle a_{i-\sigma} a_{i\sigma}\rangle = 0 . \quad (54)$$

Under these approximations Eq. (52) becomes

$$(\omega+\mu-T_0-I)\langle\langle n_{i-\sigma} a_{i\sigma}; a^{\dagger}_{\mu\sigma}\rangle\rangle_{\omega} = \langle n_{d-\sigma}\rangle \frac{\delta_{i\mu}}{2\pi} + \langle n_{d-\sigma}\rangle \sum_{l\neq i} T_{il} G^{\sigma}_{l\mu}(\omega) + \langle n_{d-\sigma}\rangle \sum_{\vec{k}} V^{*}_{\vec{k}d} e^{-i\vec{k}\cdot\vec{R}_i} G^{\sigma}_{\vec{k}\mu}(\omega) . \quad (55)$$

When we substitute the values of the Green's functions $\langle\langle n_{i-\sigma}; a^{\dagger}_{\mu\sigma}\rangle\rangle_{\omega}$ from Eq. (55) in Eqs. (11c) and (11d), Eqs. (11) acquire a closed form. By solving these equations for $G^{\sigma}_{\vec{k}\vec{k}}(\omega)$ and $G^{\sigma}_{d\vec{k}}(\omega)$ we get

$$G^{\sigma}_{\vec{k}\vec{k}}(\omega) = \left(\frac{(\omega+\mu-T_0)(\omega+\mu-T_0-I)}{(\omega+\mu-T_0-I)(1-\langle n_{d-\sigma}\rangle)} - (\epsilon_{d\vec{k}}-T_0)\right) \times (\omega+\mu-\epsilon_{\vec{k}})^{-1} G^{\sigma}_{d\vec{k}}(\omega) , \quad (56)$$

$$G^{\sigma}_{d\vec{k}}(\omega) = \frac{1}{2\pi}\left(\frac{(\omega+\mu-T_0)(\omega+\mu-T_0-I)}{\omega+\mu-T_0-I(1-\langle n_{d-\sigma}\rangle)} - (\epsilon_{d\vec{k}}-T_0) - \frac{N|V_{\vec{k}d}|^2}{\omega+\mu-\epsilon_{\vec{k}}}\right)^{-1} . \quad (57)$$

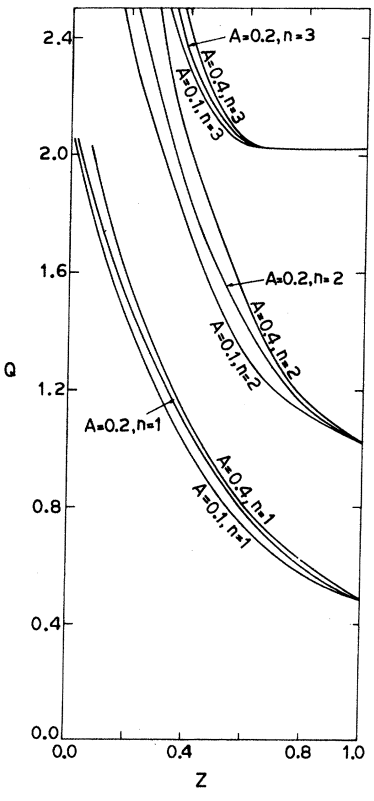

FIG. 5. Variation of the Fermi level with Z in the Hartree-Fock approximation for a finite d-band width and the square density of states for s band. Curves are plotted for $P=2.0$ and $S=0.1$.

TABLE III. Range of Z for ferromagnetic solutions for the finite width of the d band.

P	S	A	n	Z
2.0	0.1	0.1	1.0	0.05–0.4
			2.0	0.11–1.0
			3.0	0.26–1.0
		0.2	1.0	0.1 –0.4
			2.0	0.16–1.0
			3.0	0.26–1.0
		0.4	1.0	0.15–0.4
			2.0	0.26–1.0
			3.0	0.31–1.0

These Green's functions have the same singularities which are simple poles. There are three quasiparticle bands, which arise from the s band crossing and hybridizing with the two pseudo-d-bands, given by the roots of the equation

$$(\omega+\mu-T_0)(\omega+\mu-T_0-I)-(\epsilon_{d\vec{k}}-T_0) \times [\omega+\mu-T_0-I(1-\langle n_{d-\sigma}\rangle)] = 0 . \quad (58)$$

In general, the roots of the cubic equation, which determines the poles of the Green's functions, are not all real. However, we can avoid this situation by taking the limit $I\to\infty$. In this limit the upper band given by Eq. (58) is pushed out to infinity and we have only two bands to consider. When $I\to\infty$ the Green's functions $G^{\sigma}_{\vec{k}\vec{k}}(\omega)$ and $G^{\sigma}_{d\vec{k}}(\omega)$ are given by

$$G^{\sigma}_{\vec{k}\vec{k}}(\omega) = \left(\frac{\omega+\mu-T_0}{1-\langle n_{d-\sigma}\rangle} - (\epsilon_{d\vec{k}}-T_0)\right) \times (\omega+\mu-\epsilon_{\vec{k}})^{-1} G^{\sigma}_{d\vec{k}}(\omega) , \quad (59)$$

$$G^{\sigma}_{d\vec{k}}(\omega) = \frac{1}{2\pi} \times \left[\frac{\omega+\mu-T_0}{1-\langle n_{d-\sigma}\rangle} - (\epsilon_{d\vec{k}}-T_0) - \left(\frac{N|V_{\vec{k}d}|^2}{\omega+\mu-\epsilon_{\vec{k}}}\right)\right]^{-1} . \quad (60)$$

By substituting the values of $G^{\sigma}_{\vec{k}\vec{k}}(\omega)$ and $G^{\sigma}_{d\vec{k}}$ from Eqs. (59) and (60) in Eqs. (15) and (16), we obtain

$$\rho^{\sigma}_{s}(\omega) = \frac{1}{N}\sum_{\vec{k}} [B^{+}_{s\vec{k}\sigma}\delta(\omega-\tilde{\omega}^{+}_{\vec{k}\sigma}) + B^{-}_{s\vec{k}\sigma}\delta(\omega-\tilde{\omega}^{-}_{\vec{k}\sigma})] , \quad (61)$$

$$\rho^{\sigma}_{d}(\omega) = \frac{1}{N}\sum_{\vec{k}} [B^{+}_{d\vec{k}\sigma}\delta(\omega-\tilde{\omega}^{+}_{\vec{k}\sigma}) + B^{-}_{d\vec{k}\sigma}\delta(\omega-\tilde{\omega}^{-}_{\vec{k}\sigma})] , \quad (62)$$

where

$$\tilde{\omega}^{p}_{\vec{k}\sigma} = -\mu + \tfrac{1}{2}(\epsilon_{\vec{k}} + T_0 + (\epsilon_{d\vec{k}} - T_0)(1 - \langle n_{d-\sigma}\rangle) + p\{[T_0 + (\epsilon_{d\vec{k}} - T_0)(1 - \langle n_{d-\sigma}\rangle) - \epsilon_{\vec{k}}]^2 + 4N|V_{\vec{k}d}|^2(1 - \langle n_{d-\sigma}\rangle)\}^{1/2}) \quad , \tag{63}$$

$$B^{p}_{s\vec{k}\sigma} = p\left(\frac{\tilde{\omega}^{p}_{\vec{k}\sigma} + \mu - T_0 - (\epsilon_{d\vec{k}} - T_0)(1 - \langle n_{d-\sigma}\rangle)}{\tilde{\omega}^{+}_{\vec{k}\sigma} - \tilde{\omega}^{-}_{\vec{k}\sigma}}\right) , \tag{64}$$

$$B^{p}_{d\vec{k}\sigma} = p(1 - \langle n_{d-\sigma}\rangle)\frac{\tilde{\omega}^{p}_{\vec{k}\sigma} + \mu - \epsilon_{\vec{k}}}{\tilde{\omega}^{+}_{\vec{k}\sigma} - \tilde{\omega}^{-}_{\vec{k}\sigma}} \quad . \tag{65}$$

Equations (61) and (62) show that both s and d bands are split into two bands with despersion laws $\omega = \tilde{\omega}^{+}_{\vec{k}\sigma}$ and $\omega = \tilde{\omega}^{-}_{\vec{k}\sigma}$. The general form of these bands comes out to be similar to that in the Hartree-Fock approximation. Here again for zero width of the d band, the two bands are always separated by an energy gap. But in this case the two bands are separated by an asymptote at $T_0 - \mu$ instead of $T_0 - \mu + T\langle n_{d-\sigma}\rangle$ in the Hartree-Fock approximation. Again the band gap decreases as the d-band width increases and finally they overlap each other. In this case, in general, the number of states per atom for each spin in the lower band is not equal to 1. Therefore, a system having two electrons per atom will behave as a metal instead of an insulator. However, for some particular choice of parameters I, v, T_0, and α it may behave as an insulator. The number of states per atom for each spin in both the bands together is equal to $B^{+}_{s\vec{k}\sigma} + B^{-}_{s\vec{k}\sigma} + B^{+}_{d\vec{k}\sigma} + B^{+}_{d\vec{k}\sigma} = 2 - \langle n_{d-\sigma}\rangle$ instead of 2 as in the Hartree-Fock approximation. This is due to the fact that the upper band given by Eq. (58) has been pushed out to infinity.

A. Zero Bandwidth

In the zero-bandwidth case, Eqs. (61) and (62) take the form

$$\rho^{\sigma}_{s}(\omega) = N[f^{c}_{\sigma}(\omega + \mu)] , \tag{66}$$

$$\rho^{\sigma}_{d}(\omega) = (1 - \langle n_{d-\sigma}\rangle)\left|\frac{\omega + \mu - f^{c}_{\sigma}(\omega + \mu)}{\omega + \mu - T_0}\right| N[f^{c}_{\sigma}(\omega + \mu)] , \tag{67}$$

where $$f^{c}_{\sigma}(\omega) = \omega - \frac{|v|^2(1 - \langle n_{d-\sigma}\rangle)}{\omega - T_0} \quad . \tag{68}$$

Equations (66) and (67) give the average number of s and d electrons per atom for spin σ as

$$\langle n_{s\sigma}\rangle = \int_{-\infty}^{\mu} N[f^{c}_{\sigma}(\omega)]d\omega , \tag{69}$$

$$\langle n_{d\sigma}\rangle = (1 - \langle n_{d-\sigma}\rangle)^2 \int_{-\infty}^{\mu} \frac{|v|^2}{(\omega - T_0)^2} N[f^{c}_{\sigma}(\omega)]d\omega . \tag{70}$$

Above equations are used to obtain the ferromagnetic solution for square density of states. In Fig. 6, Q-versus-Z curves are plotted for three different values of S, 0.1, 0.3, 1.0. Here and in Sec. IV B we do not consider the case $n = 3$ because in this case both s and d bands are completely filled. It is found that ferromagnetic solutions are possible only for $n = 1.0$, $S = 1.0$, and Z from 0.01 to 0.12. This shows that the square density of states is less favorable to ferromagnetism than the parabolic density of states studied by Smith who found that for $n = 1$, ferromagnetic solutions are possible for $S = 1.0$ and also for $S = 0.3$. Thus the ferromagnetic solutions are influenced by the shape of the density of states. In Fig. 7 the self-consistent magnetic solutions are shown.

B. Finite Bandwidth

To consider the effect of the width of the d band on the ferromagnetic solutions, we take the d band given by Eq. (41). The densities of states $\rho^{\sigma}_{s}(\omega)$ and $\rho^{\sigma}_{d}(\omega)$ are given by

$$\rho^{\sigma}_{s}(\omega) = \frac{1}{N}\sum_{\vec{k}} |\omega + \mu - T_0 - A(1 - \langle n_{d-\sigma}\rangle)(\epsilon_{\vec{k}} - \tfrac{1}{2}\alpha)| \times \delta[(\omega - \tilde{\omega}^{+}_{\vec{k}\sigma})(\omega - \tilde{\omega}^{-}_{\vec{k}\sigma})] , \tag{71}$$

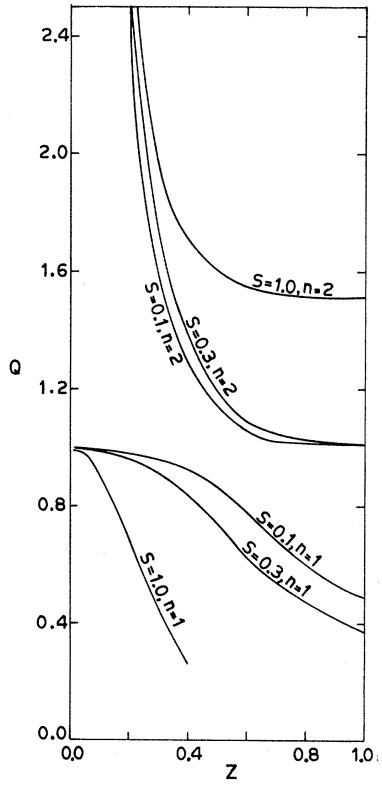

FIG. 6. Variation of the Fermi level with Z in the correlation theory for the zero d-band width and the square density of states for the s band.

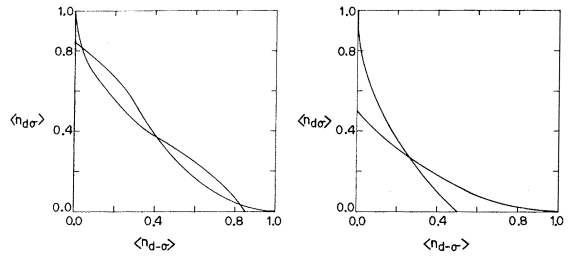

FIG. 7. Self-consistent magnetic solutions in the correlation theory for zero d-band width and the square density of states for the s band. The parameters used are (a) $n=1$, $S=1.0$, $Z=0.1$, and $Q=0.91$; (b) $n=1$, $S=1.0$, $Z=0.2$, and $Q=0.68$.

$$\rho_d^\sigma(\omega)=\frac{1}{N}\sum_{\vec{k}}(1-\langle n_{\vec{d}-\sigma}\rangle)\,|\,\omega+\mu-\epsilon_{\vec{k}}|\times\delta[(\omega-\tilde{\omega}_{\vec{k}\sigma}^{+})(\omega-\tilde{\omega}_{\vec{k}\sigma}^{-})]\,. \tag{72}$$

If we assume that $A(1-\langle n_{d-\sigma}\rangle)\neq 0$, these equations can be rewritten as

$$\rho_s^\sigma(\omega)=[A(1-\langle n_{d-\sigma}\rangle)]^{-1}\times\sum_{p=\pm}\left|\frac{\omega+\mu-T_0+\frac{1}{2}A(1-\langle n_{d-\sigma}\rangle)(\alpha-2g_\sigma^p(\omega+\mu))}{g_\sigma^+(\omega+\mu)-g_\sigma^-(\omega+\mu)}\right|\times N[g_\sigma^p(\omega+\mu)]\,, \tag{73}$$

$$\rho_d^\sigma(\omega)=\frac{1}{A}\sum_{p=\pm}\left|\frac{\omega+\mu-g_\sigma^p(\omega+\mu)}{g_\sigma^+(\omega+\mu)-g_\sigma^-(\omega+\mu)}\right|N[g_\sigma^p(\omega+\mu)]\,, \tag{74}$$

where

$$g_\sigma^p(\omega)=[2A(1-\langle n_{d-\sigma}\rangle)]^{-1}\{\omega-T_0+(1-\langle n_{d-\sigma}\rangle)\times(A\omega+\tfrac{1}{2}A\alpha)+p[(\omega-T_0-A(\omega-\tfrac{1}{2}\alpha)\times(1-\langle n_{d-\sigma}\rangle))^2+4|v|^2(1-\langle n_{d-\sigma}\rangle)^2]^{1/2}\}\,. \tag{75}$$

From (73) and (74) we obtain $\langle n_{d\sigma}\rangle$ and $\langle n_{d-\sigma}\rangle$ at absolute zero:

$$\langle n_{s\sigma}\rangle=\frac{1}{A(1-\langle n_{d-\sigma}\rangle)}\int_{-\infty}^{\mu}\sum_{p=\pm}\times\left|\frac{\omega-T_0+\frac{1}{2}A(1-\langle n_{d-\sigma}\rangle)[\alpha-2g_\sigma^p(\omega)]}{g_\sigma^+(\omega)-g_\sigma^-(\omega)}\right|\times N[g_\sigma^p(\omega)]\,d\omega\,, \tag{76}$$

$$\langle n_{d\sigma}\rangle=\frac{1}{A}\int_{-\infty}^{\mu}\sum_{p=\pm}\left|\frac{\omega-g_\sigma^p(\omega)}{g_\sigma^+(\omega)-g_\sigma^-(\omega)}\right|N[g_\sigma^p(\omega)]\,d\omega\,. \tag{77}$$

Equations (76) and (77) are analyzed to get the magnetic solutions. For the zero width of the d band the case of parabolic density of states was analyzed by Smith and square density of states by us in Sec. III. We consider here both the square and the parabolic density of states to get an idea of the change of the magnetic solutions with the d-band width. In Figs. 8 and 9 the plots of Q versus Z are given for the square and parabolic density of states, respectively. We have taken $A=0.1$, 0.2, and 0.4 and $S=1.0$. A search for magnetic solutions shows that the ferromagnetic solutions are not possible for any of these curves.

V. METAL-NONMETAL TRANSITION

In this section we investigate the role of the s-d interaction in metal-nonmetal transition. We restrict our treatment to the case $I=0$. In this case Eqs. (11) can be solved exactly to give the s and d electron Green's functions.

$$G_{\vec{k}\vec{k}}^\sigma(\omega)=\frac{(\omega-E_{\vec{k}})/2\pi}{(\omega-E_{\vec{k}})(\omega-E_{\vec{d}\vec{k}})-N|V_{\vec{k}d}|^2}\,, \tag{78}$$

$$G_{\vec{d}\vec{k}}^\sigma(\omega)=\frac{(\omega-E_{\vec{k}})/2\pi}{(\omega-E_{\vec{k}})(\omega-E_{\vec{d}\vec{k}})-N|V_{\vec{k}d}|^2}\,. \tag{79}$$

These Green's functions are independent of the spin index σ. By substituting the values of $G_{\vec{k}\vec{k}}^\sigma(\omega)$ and $G_{\vec{d}\vec{k}}^\sigma(\omega)$ from (78) and (79) in Eqs. (15) and (16),

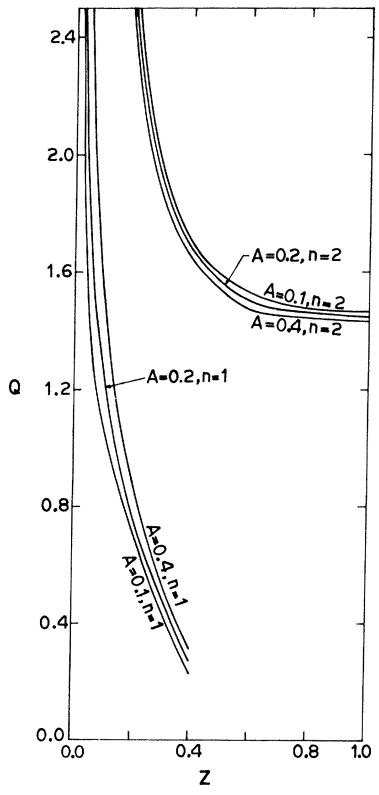

FIG. 8. Variation of the Fermi level with Z in the correlation theory for a finite d-band width and the square density of states for the s band. Curves are plotted for $S=1.0$.

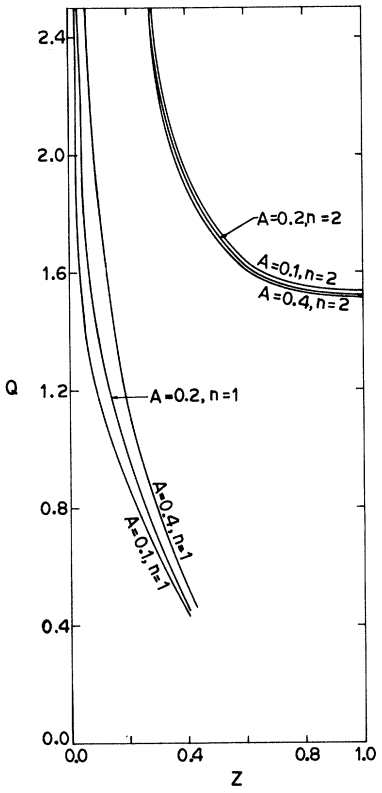

FIG. 9. Variation of the Fermi level with Z in the correlation theory for a finite d-band width and the parabolic density of states for the s band. Curves are plotted for $S = 1.0$.

we obtain

$$\rho_s(\omega)=\frac{1}{N}\sum_{\vec{k}}[A^{+}_{s\vec{k}}\delta(\omega-\omega^{+}_{\vec{k}})+A^{-}_{s\vec{k}}\delta(\omega-\omega^{-}_{\vec{k}})] \quad (80)$$

and

$$\rho_d(\omega)=\frac{1}{N}\sum_{\vec{k}}[A^{+}_{d\vec{k}}\delta(\omega-\omega^{+}_{\vec{k}})+A^{-}_{d\vec{k}}\delta(\omega-\omega^{-}_{\vec{k}})] \ , \quad (81)$$

where the hybrid bands $\omega^{\pm}_{\vec{k}}$ are given by

$$\omega^{\pm}_{\vec{k}}=\tfrac{1}{2}\{E_{\vec{k}}+E_{d\vec{k}}\pm[(E_{d\vec{k}}-E_{\vec{k}})^2+4N|V_{\vec{k}d}|^2]^{1/2}\} \quad (82)$$

and $$A^{p}_{s\vec{k}}=p(\omega^{p}_{\vec{k}}-E_{d\vec{k}})/(\omega^{+}_{\vec{k}}-\omega^{-}_{\vec{k}}) \ , \quad (83)$$

$$A^{p}_{d\vec{k}}=p(\omega^{p}_{\vec{k}}-E_{\vec{k}})/(\omega^{+}_{\vec{k}}-\omega^{-}_{\vec{k}}) \ . \quad (84)$$

From (83) and (84) we have $A^{-}_{s\vec{k}}+A^{-}_{d\vec{k}}=1$. This shows that the number of states in the lower band is equal to 1 for each spin. If we choose a system with two electrons per atom in s and d band together, the system will behave as a nonmetal if there is a gap between the lower and upper hybrid bands; otherwise it will behave as a metal. A metal-nonmetal transition occurs when the band gap becomes zero. Under the assumption (41) for $\epsilon_{d\vec{k}}$, we obtain from (82) the following condition for zero band gap:

$$(A+1)^2S^2-A[\tfrac{1}{4}A(A+2)B^2+B-1]=0 \ , \quad (85)$$

where $B=\alpha/T_0=1/Z$. Equation (85) contains three parameters. By fixing a particular parameter, one can plot a transition curve for the remaining two parameters. In Figs. 10–12 we have plotted S-B, S-A, and B-A curves for different values of A, B, and S, respectively. In Figs. 10 and 11, the regions above and below a transition curve correspond to nonmetallic and metallic behaviors, respectively, while in Fig. 12 the situation is just the reverse. These curves show that for a particular choice of values of S and B we get a critical value of A at which the transition from the nonmetallic to the metallic state occurs. When we apply pressure on a nonmetallic substance, the lattice parameter decreases, and consequently A increases; therefore, a transition from nonmetallic to metallic state should occur at a critical pressure when A crosses the critical value determined by the choice of S and B. But it should be remembered that S increases as we increase the pressure, because the overlapping of s and d wave functions increases owing to compression of the

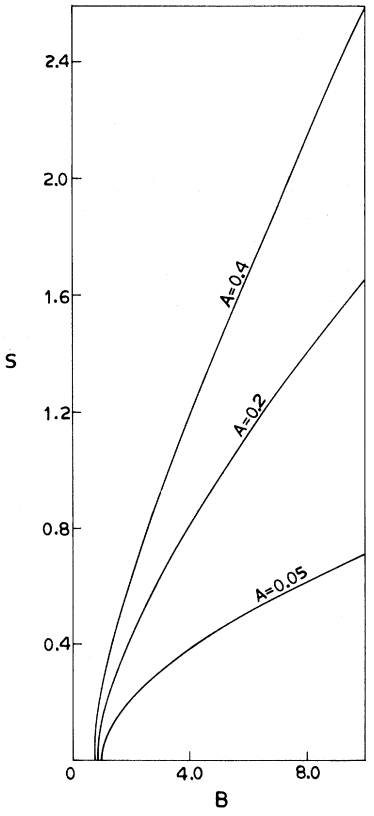

FIG. 10. S-B curves for different values of A.

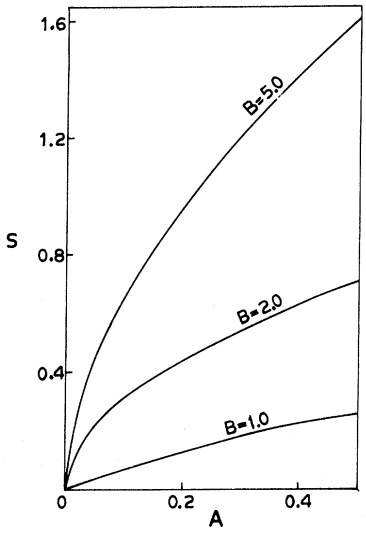

FIG. 11. S-A curves for different values of B.

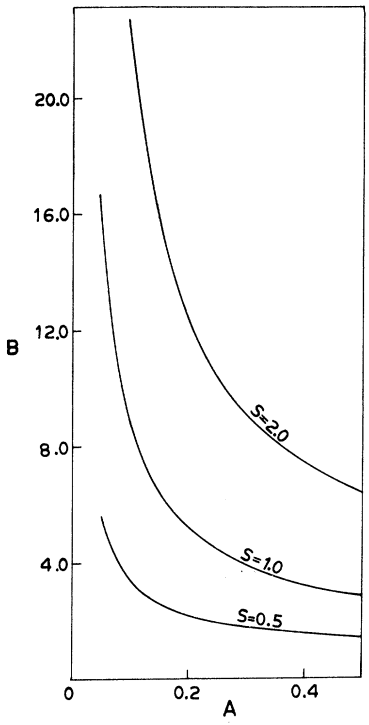

FIG. 12. B-A curves for different values of S.

lattice. Figure 11 clearly shows that this increase in S does not favor the nonmetal-metal transition. Thus, the s-d interaction opposes the pressure induced nonmetal-metal transition predicted by Mott.[12] This kind of approach may explain the difficulty of observing metal-nonmetal transition under pressure.[13]

VI. CONCLUSIONS

The results of the correlation theory for ferromagnetic solutions are in marked disagreement with those of the Hartree-Fock theory. In the Hartree-Fock theory, as the strength of s-d hybridization increases, the tendency towards ferromagnetism decreases, while the reverse is true for the correlation theory. In the Hartree-Fock theory the ferromagnetic solutions are possible for $n = 1$, 2, 3, while in the correlation theory, ferromagnetic solutions are possible only for $n = 1$. In both the theories, the tendency towards ferromagnetism decreases as the bandwidth increases. Our conclusion that ferromagnetism is possible for square density of states[14] disagrees with Hubbard's theory which predicts that for this type of density of states ferromagnetism is not possible. Furthermore, in correlation theory tendency towards ferromagnetism increases as the hybridization between the s and d bands increases. This shows the importance of s-d hybridization in the correlation theory of ferromagnetism. In the Hartree-Fock theory the strength of the intraatomic interaction favors ferromagnetism. It is also shown that the s-d interaction stiffens the conditions for the pressure induced metal-nonmetal transitions.

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[14]Here we have taken the form of the d band same as that of s band, therefore the form of the density of states should be the same for both the bands. Since a square density of states is taken for s band, we shall have a square density of states for d band also.