Two-band model for the magnetism of iron

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We introduce a two-band model for the magnetism of Fe and report results in fairly good agreement with many experimental facts both at low and high temperatures. One band is narrow and degenerate, representing the "quasilocalized" electrons. The second one is a wide band containing very few itinerant electrons. The occupation of these bands is suggested by positron annihilation data and the observed saturation moment. The one-particle excitations and the transverse dynamical susceptibility are calculated within the Hartree-Fock and the random-phase approximations, respectively. An exchange coupling between electrons of both bands plays a crucial role in determining the magnetic state of the system, as evidenced in the derived modified Stoner criterion. On the other hand, an effective interatomic exchange coupling between electrons of the narrow band is necessary for the spin-wave stiffness constant to assume the extrapolated "experimental value" at zero temperature. Moreover, an excellent fitting of the temperature dependence of the static paramagnetic susceptibility is obtained. The results are analyzed in view of Stearns's ideas concerning the origin of the magnetism of Fe.

I. INTRODUCTION

The origin of magnetism in transition metals and compounds has been the core of a long-standing controversy in the theory of magnetic solids.[1] Today everyone agrees that some degree of itinerancy must be granted to the d electrons in order to explain many basic experimental facts, such as the saturate nonintegral number of Bohr magnetons per atom. However, the very complex nature of the valence states has prevented as yet a complete understanding of the dominant mechanisms underlying the magnetic properties of these materials. Very few attempts at first-principles calculations exist,[2] and these are limited to describing low-temperature properties, such as the spin-wave dispersion relation. An issue which has challenged first-principles theories is the observation[3] of propagating spin waves above T_c.

The more recent major theoretical efforts to overcome the difficulties encountered by the Stoner theory of itinerant ferromagnetism to explain the finite-temperature properties are in the direction of improving the treatment of electron-electron correlation.[4,5] The prototype model of these studies is the Hubbard model[6] and the main assertion is that the magnetism of transition metals is due to strong correlation effects in narrow d bands, the driving force being the intra-atomic Coulomb interaction. However, since a long time past, many authors[7-10] insist that a full explanation of the occurrence of magnetism in these systems must properly account for the relative importance of Hund's rule coupling, of interatomic interactions and of the nature of the d states in the fivefold degenerate d bands partially hybridized with s bands. In this context we shall introduce a two-band model for the magnetism of Fe and report results in fairly good agreement with many experimental facts both at low and high temperatures. Our findings evidence that the origin of magnetism in Fe may result from a cooperative effect much in accord with the views put forward by Stearns[8] in the last decade.

According to Stearns's ideas[8] the ferromagnetism of Fe obeys two conditions. The first is that the intra-atomic exchange interaction splits the flat E_g bands into spin-up (below the Fermi level E_F) and spin-down (above E_F) bands and a localized moment develops. The second condition for ferromagnetism is met by turning on the exchange interaction between the itinerant electrons belonging to a paraboliclike T_{2g} band and the "localized" electrons of the E_g bands. Thus ferromagnetism would arise from the Ruderman-Kittel-Kasuya-Yosida (RKKY)-type indirect coupling of the local moments through the itinerant d electrons. RKKY-type calculations predict that about 5% of the $3d$ electrons are in itinerant bands and 95% are in d bands which are sufficiently narrow that they can be considered localized.

Obviously, this is a quite naive scheme to build up a localized moment in Fe. In particular, at arbitrary points of the Brillouin zone, the d-symmetry part of the wave function has both nonnegligible E_g and T_{2g} components.[2] Other aspects have been discussed by Mattis,[11] who also emphasizes the need of two dissimilar bands—one very narrow and the other delocalized—as the simplest band model suitable to describe the magnetic properties of Fe. In any event, the above scheme illustrates the main physical point of the proposal: existence of very few "almost free" itinerant electrons playing an important role in polarizing the majority and more localized electrons occupying the relatively flat portions of the band structure. This

picture[8] was motivated by results of band-structure calculations,[12] and of de Haas–van Alphen,[13] spin-polarization[14] and hyperfine measurements.[15] In fact, by analyzing the results of their band-structure calculation, Duff and Das[12] suggested an identical proposal for the origin of iron's ferromagnetism. Recently, positron annihilation experiments[16] across the transition metal series have provided a deep microscopic probe of the itinerant versus localized dichotomy of the d electrons in these materials. For Fe the annihilation rates suggest 0.5 itinerant and 6 localized d electrons per atom.

In this paper, however, we make no *ad hoc* hypothesis concerning spin localization, which has suffered much criticism when dealing with itinerant magnets. Rather, the main goal here is to present a full band model based upon the above-described ideas, subjected to a parametrization suitable to describe the magnetic properties of Fe.

The model Hamiltonian is presented in the next section. In Sec. III we derive the basic equations and report the numerical results. The main conclusions are stated in Sec. IV.

II. MODEL HAMILTONIAN

The model Hamiltonian may be written in the form

$$H=\sum_{i,j,\sigma,\alpha} T_{ij}^{\alpha} C_{i\sigma}^{\alpha\dagger} C_{j\sigma}^{\alpha} + \tfrac{1}{2} \sum_{i,\sigma,\alpha} U_{\alpha} n_{i\sigma}^{\alpha} n_{i,-\sigma}^{\alpha} - 2J_{IL} \sum_{i} \mathbf{S}_i^I \cdot \mathbf{S}_i^L - 2J \sum_{i<j} \mathbf{S}_i^L \cdot \mathbf{S}_j^L , \tag{1}$$

where $C_{i\sigma}^{\alpha}$ ($C_{i\sigma}^{\alpha\dagger}$) is the annihilation (creation) operator for an electron of spin σ at the site i and band α, $n_{i\sigma}^{\alpha}$ and $\mathbf{S}_i^{\alpha}$ are the occupation number and spin operators of these electrons, respectively, T_{ij}^{α} are the Wannier representation of the electron bands, U_{α} are the intra-atomic intraband Coulomb couplings, J_{IL} is the exchange coupling between itinerant electrons of a wide band I of width Δ (quasi-free-electron states) and "quasi-localized" electrons of a narrow degenerate band L of width l (flat parts of the d bands), and J is the inter-atomic exchange coupling between electrons of the narrow band.

A most important feature in our band model is that both the itinerant and quasilocalized electrons are governed by the same Fermi level, a characteristic to be preserved in itinerant d-electron systems. Our viewpoint is that the parameters of our model Hamiltonian are to be considered effective ones, already renormalized by correlation, screening effects, etc., in such a way that if all physical relevant couplings are present we are allowed to use Hartree-Fock (HF) approximation and the random-phase approximation (RPA) to calculate the one-particle excitations and the dynamic response of the system, respectively. Clearly, this is the simplest way of getting effective couplings for the theory and many important features of the model may not appear when using this procedure.

In closing this section we should point out that when the width of the narrow degenerate band approaches zero, with the effective U_L satisfying $U_L < l$,[17] the quasilocalized electrons are strictly localized; an ($S=1$)-localized spin then emerges and our model becomes identical to that of Edwards.[9]

III. BASIC EQUATIONS AND NUMERICAL RESULTS

In the HF approximation the one-particle Green's functions of the system are given by

$$G^{\alpha}(\mathbf{k},\omega)=\frac{1}{2\pi(\omega-\omega_{\mathbf{k}\sigma}^{\alpha})} , \tag{2}$$

where $\omega_{k\sigma}^{\alpha}$ are the one-particle excitations of electrons in the bands I and L:

$$\omega_{\mathbf{k}\sigma}^{I}=\epsilon_{\mathbf{k}}^{I}+U_I\langle n_{-\sigma}^{I}\rangle-\frac{J_{IL}}{2}(\langle n_{\sigma}^{L}\rangle-\langle n_{-\sigma}^{L}\rangle) , \tag{3}$$

$$\omega_{k\sigma}^{L}=\epsilon_{\mathbf{k}}^{L}+U_L\langle n_{-\sigma}^{L}\rangle-\frac{J_{IL}}{2}(\langle n_{\sigma}^{I}\rangle-\langle n_{-\sigma}^{I}\rangle) - \frac{J(0)}{2}(\langle n_{\sigma}^{L}\rangle-\langle n_{-\sigma}^{L}\rangle) , \tag{4}$$

where $\epsilon_{\mathbf{k}}^{\alpha}$ are the noninteracting electron bands, $J(\mathbf{q})=J\sum_{\delta}e^{i\mathbf{q}\cdot\delta}$, with δ being vectors join first neighbors of a bcc lattice, and $\langle n\rangle$ are the average number of electrons per atom. To simplify the calculations we assume paraboliclike bands and the effective-mass approximation, i.e.,

$$\epsilon_{\mathbf{k}}^{I}=\hbar^2k^2/2m_I^{*} , \tag{5}$$

$$\epsilon_{\mathbf{k}}^{L}=T_0-(l/2)+(\hbar^2k^2/2m_L^{*}) , \tag{6}$$

where T_0 fixes the position of the L band relative to the I band. Furthermore, we assume one electron state in the band I and two in the degenerate band L; thus one has as the effective density of states

$$\eta_{\sigma}^{I}(\omega)=(3/2\Delta^{3/2})(\omega-\omega_{0\sigma}^{I})^{1/2} , \tag{7}$$

$$\eta_{\sigma}^{L}(\omega)=(3/l^{3/2})(\omega-\omega_{0\sigma}^{L})^{1/2} , \tag{8}$$

where $\omega_{0\sigma}^{\alpha}\equiv\omega_{k=0,\sigma}^{\alpha}$ are the energy positions at the bottoms of the bands. The assumptions of rigid band splitting and paraboliclike bands oversimplify the actual electronic structure,[2,18] but turn the computational problem feasible. On the other hand, the results can teach us about the relevance of the details of the band structure in determining the magnetic properties of the system.

Our values for

$$\langle n^{\alpha}\rangle=(1/N)\sum_{\mathbf{k}\sigma}\langle n_{\mathbf{k}\sigma}^{\alpha}\rangle , \tag{9}$$

i.e., $\langle n^I\rangle=0.5$ and $\langle n^L\rangle=2.0$, are taken from the positron annihilation data[16] in Fe. The remaining[16] four electrons are assumed to belong to full bands and are not considered in our analysis. From the paramagnetic solution at $T=0$ we find the relation

$$m_I^{*}\Delta=m_L^{*}l=\left(\frac{9\pi^2}{\sqrt{2}}\right)^{2/3}\left(\frac{\hbar}{a}\right)^2 , \tag{10}$$

where a is the lattice constant of bcc Fe, and the value of T_0 is fixed. In the $T=0$ ferromagnetic state (see Fig. 1) we take $\sum_{\sigma}\sigma(\langle n_{\sigma}^{I}\rangle+\langle n_{\sigma}^{L}\rangle)=2.2$ and $\langle n_{\downarrow}^{L}\rangle=0$, result-

ing $\langle n_{\uparrow}^{L}\rangle=2.0$, $\langle n_{\uparrow}^{I}\rangle=0.35$, and $\langle n_{\downarrow}^{I}\rangle=0.15$. Using the last two values for $\langle n_{\sigma}^{I}\rangle$ we obtain the following relations:

$$\mu_F=0.5[(0.35)^{2/3}+(0.15)^{2/3}]\Delta+0.25U_I\ , \tag{11}$$

$$J_{IL}=0.5[(0.35)^{2/3}-(0.15)^{2/3}]\Delta-0.10U_I\ . \tag{12}$$

The parameters must be such to place the Fermi level μ_F above the $L\uparrow$ band in the $T=0$ ferromagnetic state.

The transverse dynamical susceptibility of the system is defined in terms of the total spin Green's function,

$$\chi_{-+}(\mathbf{q},\omega)=\langle\langle S_{\mathbf{q}}^{-};S_{\mathbf{q}}^{+}\rangle\rangle_{\omega}\ , \tag{13}$$

where $\mathbf{S}_{\mathbf{q}}=\sum_i e^{i\mathbf{q}\cdot\mathbf{R}_i}\,\mathbf{S}_i$ and $\mathbf{S}_i=\mathbf{S}_i^{I}+\mathbf{S}_i^{L}$. In the RPA approximation we obtain the following Green's functions:

$$\langle\langle S_I^{-}(\mathbf{q});S_I^{+}(\mathbf{q})\rangle\rangle_{\omega}=\frac{[\chi_{-+}^{L}(\mathbf{q},\omega)]^{-1}}{[\chi_{-+}(\mathbf{q},\omega)]^{-1}[\chi_{-+}^{L}(\mathbf{q},\omega)]^{-1}-J_{IL}^{2}}\ , \tag{14}$$

$$\langle\langle S_I^{-}(\mathbf{q});S_L^{+}(\mathbf{q})\rangle\rangle_{\omega}=\frac{J_{IL}}{[\chi_{-+}(\mathbf{q},\omega)]^{-1}[\chi_{-+}^{L}(\mathbf{q},\omega)]^{-1}-J_{IL}^{2}}\ , \tag{15}$$

and $\langle\langle S_L^{-}(\mathbf{q});S_L^{+}(\mathbf{q})\rangle\rangle_{\omega}$ and $\langle\langle S_L^{-}(\mathbf{q});S_I^{+}(\mathbf{q})\rangle\rangle_{\omega}$ are obtained from Eqs. (14) and (15), by the replacement $I\leftrightarrow L$, respectively, where

$$[\chi_{-+}^{I}(\mathbf{q},\omega)]^{-1}=[\chi_{-+}^{0I}(\mathbf{q},\omega)]^{-1}-U_I\ , \tag{16}$$

$$[\chi_{-+}^{L}(\mathbf{q},\omega)]^{-1}=[\chi_{-+}^{0L}(\mathbf{q},\omega)]^{-1}-[U_L+J(\mathbf{q})]\ , \tag{17}$$

and

$$\chi_{-+}^{0\alpha}(\mathbf{q},\omega)=\frac{1}{N}\sum_{\mathbf{k}}\frac{(\langle n_{\mathbf{k}+\mathbf{q},\downarrow}^{\alpha}\rangle-\langle n_{\mathbf{k},\uparrow}^{\alpha}\rangle)}{(\omega+\epsilon_{\mathbf{k}}^{\alpha}-\epsilon_{\mathbf{k}+\mathbf{q}}^{\alpha}-\Delta_{\alpha})}\ , \tag{18}$$

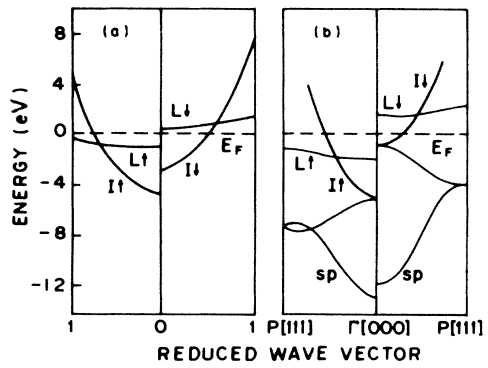

FIG. 1. (a) Sketch of the ferromagnetic ground state: $\Delta=10$ eV, $l=0.88$ eV, $U_I=0.2$ eV, $U_L=0.307$ eV, $J_{IL}=1.18$ eV, and $J=0.030$ eV. The exchange splitting of the L band is 1.31 eV and that of the I band is 2.2 eV. In this figure, $\mu_F=0$. (b) Sketch of the band structure of Fe along the Γ-P direction by Duff and Das (Refs. 12 and 8).

with $\Delta_{\alpha}=\omega_{0\downarrow}^{\alpha}-\omega_{0\uparrow}^{\alpha}$ being the exchange splittings of the bands.

From the equations above, we have

$$\chi_{-+}(\mathbf{q},\omega)=\frac{[\chi_{-+}^{I}(\mathbf{q},\omega)]^{-1}+[\chi_{-+}^{L}(\mathbf{q},\omega)]^{-1}+2J_{IL}}{[\chi_{-+}^{I}(\mathbf{q},\omega)]^{-1}[\chi_{-+}^{L}(\mathbf{q},\omega)]^{-1}-2J_{IL}^{2}}\ . \tag{19}$$

When $J_{IL}=0$ the total susceptibility is the sum of the susceptibilities of the noninteracting bands. From Eq. (19) we can obtain the spin-wave excitations, the critical temperature, and the spin contribution to the uniform static paramagnetic susceptibility.

From the poles of $\chi_{-+}(\mathbf{q},\omega)$ we derive two spin-wave branches: one optic and one acoustic in accord with the two-band solution of Yamada and Schimizu.[19] The stiffness constant of the acoustical spin wave, $\omega_{\mathrm{ac}}=Dq^2$, is found to be

$$D=\frac{1}{(\Delta n^{I}+\Delta n^{L})}\left[Ja^{2}(\Delta n^{L})^{2}+\frac{1}{3N}\sum_{\mathbf{k},\alpha}\left[\tfrac{1}{2}(n_{\mathbf{k},\uparrow}^{\alpha}+n_{\mathbf{k},\downarrow}^{\alpha})\nabla^{2}\epsilon_{\mathbf{k}}^{\alpha}-\frac{(n_{\mathbf{k}\uparrow}^{\alpha}-n_{\mathbf{k}\downarrow}^{\alpha})}{\Delta\alpha}(\nabla\epsilon_{k}^{\alpha})^{2}\right]\right]\ , \tag{20}$$

where $\Delta n^{\alpha}=n_{\uparrow}^{\alpha}-n_{\downarrow}^{\alpha}$. Similarly to Yamada and Schimizu estimates for nickel,[19] we found that the presence of the first term in Eq. (20), due to the interatomic contribution, is essential to satisfy the spin-wave criterion of ferromagnetic stability at $T=0$, namely $D>0$. We take $D=314$ meV Å^2, suggested by Stringfellow[20] as a good extrapolated value of D at $T=0$.

The modified Stoner criterion of ferromagnetic stability, obtained from the pole of $\chi_{-+}(0,0)$, reads

$$[1-U_I\chi^{I}(0,0)\,|_{T_c}]\{1-[U_L+J(0)]\chi^{L}(0,0)\,|_{T_c}\}-J_{IL}^{2}\chi^{I}(0,0)\,|_{T_c}=0\ , \tag{21}$$

where

$$\chi^{\alpha}(0,0)\,|_{T}\equiv\chi_{-+}^{0\alpha}(0,0)\,|_{T}=\int d\omega_{\mathbf{k}\sigma}^{\alpha}\eta(\omega_{\mathbf{k}\sigma}^{\alpha})\left|\frac{\partial f(\omega_{\mathbf{k}\sigma}^{\alpha})}{\partial\omega_{\mathbf{k}\sigma}^{\alpha}}\right|_{T}\ , \tag{22}$$

$f(\omega_{\mathbf{k}\sigma}^{\alpha})\equiv\langle n_{\mathbf{k}\sigma}^{\alpha}\rangle=[1+\exp\beta(\omega_{\mathbf{k}\sigma}^{\alpha})-\mu(T)]^{-1}$ is the Fermi distribution function and $\mu(T)$ is the chemical potential. At the transition temperature, $T_c=1044$ K, where $\langle n_{\uparrow}^{L}\rangle=\langle n_{\downarrow}^{L}\rangle=1.0$ and $\langle n_{\uparrow}^{I}\rangle=\langle n_{\downarrow}^{I}\rangle=0.25$, $\mu(T_c)$ is calculated from the condition

$$1=\int_{\omega_{0\sigma}^{L}}^{\omega_{0\alpha}^{L}+1}d\omega_{\mathbf{k}\sigma}^{L}\eta(\omega_{\mathbf{k}\sigma}^{L})f(\omega_{\mathbf{k}\sigma}^{L})\,|_{T_c}\ . \tag{23}$$

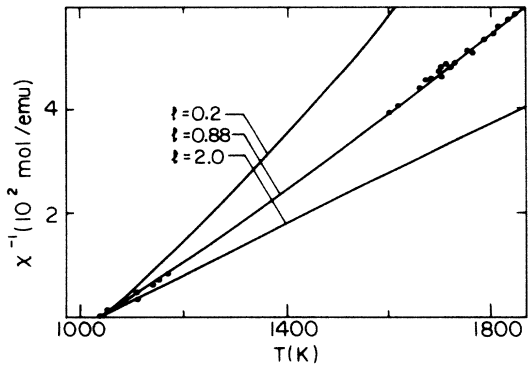

FIG. 2. Calculated temperature dependence of the static paramagnetic susceptibility for Fe: $\Delta=10$ eV, $U_I=0.2$ eV, and $J_{IL}=1.08$ eV; the other parameters are listed in Table II according to the value of l. Experimental values in bcc Fe are indicated by ● (after Ref. 23).

Some comments regarding the modified Stoner criterion, Eq. (21), are in order. If only the L band exists it reduces to the usual Stoner criterion with an interatomic contribution. In this case if the density of states at the Fermi level is sufficiently high, one may obtain a finite T_c for a reasonable value of $U_L+J(0)$. However, this is practically impossible for the I band alone. For the wide band to magnetize the exchange Hund's rule coupling J_{IL} is crucial.[21] Therefore, if the high mobile electrons appearing in the de Haas–van Alphen experiments are in fact d electrons, as suggested by Stearns,[8] some sort of RKKY-type interaction (or Hund's rule exchange) may indeed play an important role in orienting the quasilocalized electrons.

Finally, the spin contribution to the uniform static paramagnetic susceptibility may be obtained from

$$\chi_s=\tfrac{1}{2}g^2\mu_B^2\chi_{-+}(0,0)\,, \tag{24}$$

where $\chi_{-+}(0,0)$ is given by Eq. (19) for $\mathbf{q}=\omega=0,\chi^{\alpha}(0,0)\,|_T$ is defined by Eq. (22) and $\mu(T)$ is calculated from Eq. (23) for arbitrary T. The total static paramagnetic susceptibility,

$$\chi=\chi_s+\chi_{\rm orb} \tag{25}$$

includes an orbital contribution which has been estimated by Yasui *et al.*[22] of the order of $\chi_{\rm orb}\simeq 7\times10^{-5}$ emu/mol.

The numerical calculation was based on Eqs. (21)–(23) to calculate T_c and on the fitting of the temperature dependence of the paramagnetic susceptibility χ,[23] Eqs. (24) and (25) (see Fig. 2). We take $U_I=0.2$ eV, but it is rather irrelevant to any of our qualitative conclusions.

TABLE I. Dependence of D with l and U_L when $J=0$.

l (eV)	U_L (eV)	D (eV Å^2)
2.00	1.289	−0.673
0.90	0.560	−0.139
0.88	0.547	−0.135
0.70	0.429	−0.097
0.50	0.302	−0.054
0.20	0.137	0.060

TABLE II. Collection of parameters satisfying the low-temperature properties and $T_c=1044$ K.

l (eV)	U_L (eV)	J (eV)
2.00	0.762	0.066
0.90	0.318	0.030
0.88	0.307	0.030
0.70	0.209	0.027
0.50	0.105	0.025
0.20	0.001	0.017

We could just as well set it as zero. When $J=0$, it is not possible to obtain the "experimental value" of D (see Table I). By imposing its correct value, a number of collections of parameters was found to satisfy the low-temperature properties and $T_c=1044$ K (see Table II). The somewhat high effective values of J may be understood as an indirect effect of the RKKY-type interaction not properly computed in the present approximation. The "best values" of Δ and J_{IL}, not listed in Tables I and II, were $\Delta=10$ eV and $J_{IL}=1.08$ eV. An excellent fitting of the temperature dependence of χ is found when $l=0.88$ eV, $\Delta=10$ eV, $U_L=0.307$ eV, $J_{IL}=1.08$ eV, and $J=0.030$ eV (see Fig. 2).

The "best values" of l and Δ are surprisingly near Stearns's suggestions,[8] $l=0.7$ eV and $\Delta=10$ eV. The crucial feature to obtain a good fitting of χ is indeed the width of the L band (see Fig. 2). A correct behavior for χ is obtained when the L band is sufficiently narrow so that at such temperatures the statistics cause a response which is intermediate between a Curie-type behavior and a temperature-independent Pauli susceptibility. The corresponding effective value of U_L is rather small but fortunately it satisfies the condition[17] $U_L<l$, otherwise the use of the Hartree-Fock approximation and random-phase approximation would be inconsistent. It should be understood as indicative of strong correlation effects in such narrow d bands, though a greater value may be obtained if hybridization with s bands is invoked to satisfy the spin-wave criterion of ferromagnetism, as recently suggested by Muniz.[24] Finally, for comparison, we have sketched in Fig. 1(b) the band structure of ferromagnetic Fe along the Γ-P direction, as calculated by Duff and Das.[12,8] It is interesting to observe that the resulting "magnetic bands" of our simple model, Fig. 1(a), resemble some features of the corresponding ones of this more elaborated one-electron calculation. Deviations of this simple behavior occur along other directions in the Brillouin zone.[12,8]

IV. CONCLUSIONS

It is rather gratifying that the results obtained using the simple two-band model presented in this paper are in accord with many experimental facts both at low and high temperatures. The main feature of the model is the existence of a degenerate narrow band, representing the electrons occupying the flat portions of the d bands ("quasilocalized" electrons), and of a wide band containing very few quasifree electrons (itinerant electrons). An exchange

coupling between electrons of both bands plays a crucial role in determining the magnetic state of the system, as clearly evidenced in the derived modified Stoner criterion, Eq. (16). On the other hand, the presence of an effective interatomic exchange coupling between electrons of the narrow band is necessary for the spin-wave stiffness constant to assume the extrapolated "experimental value" at $T=0$, as found in other two-band calculations.[19] Moreover, an excellent fitting of the temperature dependence of the static paramagnetic susceptibility is obtained. The results give support to the ideas of Stearns[15] concerning the origin of the magnetism of Fe.

In conclusion we should remark that several simplified assumptions have been made in order to build up the model and to perform the calculations. Nevertheless, since the results are in accord with many experimental facts we tend to conclude that the proposed model contains some of the relevant features underlying the magnetic properties of Fe, particularly those needed to describe the thermodynamic ones. Dynamic properties,[2,3] on the other hand, seem to be much more sensitive to details of the electronic structure and correlation effects. In these cases, first-principles calculations and more elaborate treatments of correlations have to be implemented for a quantitative comparison with the available experimental data.

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