A0004/78

JAN,1978

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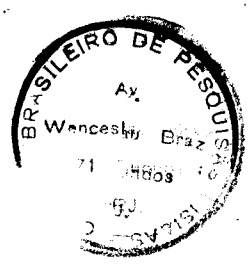

# A THEORETICAL STUDY OF HYPERFINE FIELDS PF RARE EARTH IMPURITIES IN TRANSITION HOSTS*

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* To be published in Physical Review B.

** Under a grant from International Atomic Energy Agency (IAEA) during a stay at the Laboratoire de Physique des Solides (Orsay), in 1976.

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†† Under a grant from CNPq (Brazilian Government).

ABSTRACT

We study theoretically the hyperfine field at the nucleus of a rare earth impurity embedded in a transition host. Thys system is a limiting case of the Blandin-Campbell problem, namely, that of the hyperfine field at a non magnetic impurity site in a metallic matrix doped with a magnetic impurity at a distance $R_o$ (Heusler alloys).

In the case we study, both the polarizing spin and the charge impurity potential collapse into the same site (i.e., $R_o = 0$). Furthermore, one must consider a more complicated band structure: an s- and d- character conduction band.

We perform numerical computations for a number of model band structures taking into account the two-band nature of the transition metals and treating the exchange couplings of the impurity f-spin with the s- and d- electron gas to first order in perturbation. The s- and d- hyperfine contributions are calculated in terms of local magnetic responses $\bar{\chi}^{\lambda\mu}(0)$, $(\lambda,\mu = s,d)$, which incorporates the host band structure, charge potential and local correlations, and ratios between the hyperfine parameters $A_{cp}$ and $A(Z)$.

We find that the s- contribution to the hyperfine field may change sign with the impurity potential difference between rare earth impurity and the matrix. However, the d- contribution does not; as it is the dominant one, the total hyperfine field remains always positive (negative) throughout the transition metal series depending on whether the exchange coupling $J^{(d)}$ between the d- electron gas and the f- local spin is negative (positive).

Our theory may be useful to extract information on the order parameter in certain spin glass systems from hyperfine field measurements.

Our theoretical results are compared with some available experimental data and further systematic experimental studies are suggested including spin glass systems.

## I - INTRODUCTION

The hyperfine field at s-p impurities in ferromagnetic metals are systematically negative for elements in the first half of an s-p series and positive in the second half [1].

The same behavior is observed for hyperfine field at the s-p site Y in the Heusler alloys $X_L MnY$ [2,3]. It has been suggested [4] that this behavior can be understood on the basis of a generalization of the Ruderman-Kittel-Kasuya-Yosida (RKKY) approach, to an electron gas with a strong and localized perturbation acting at the Y site.

Changes of sign occur also in the case of transition impurities embedded in rare-earth hosts, like Gd [5].

In the n-d transition series, dissolved in these systems, the holes in the d-band are progressively emptied producing thereby a change of sign in the hyperfine field [5].

In ref. [4], the calculation of the polarization at a non-magnetic site in a ferromagnetic alloy, rests on the following basic assumptions. The conduction electrons are considered as free-electron like. A non-magnetic normal impurity placed at the origin introduces a spin independent spherical potential $V_o(r)$ giving rise to phase shifts $\delta_\ell$, the scattering associated to this potential being treated exactly. A magnetic impurity located at $R_0 \neq 0$ interacts with the conduction electrons through the effective s-d exchange $H_{exch} = -J\delta(r-R_o)\, s.S$ (this being an essential assumption for the case of Heusler alloys). The spin-dependent potential is treated within the Born approximation. This calculation gives for the magnetization at the origin [4]

$$m_{R_o}(r=0) = -\frac{K_F}{2\pi^2} J\Omega_o \langle S^z \rangle |\phi_{K_F}(0)|^2 \frac{\cos(2K_F R_o + 2\delta_o{}^F)}{R_o^3} \qquad (1.1)$$

where $|\phi_{K_F}(o)|^2$ is the one electron wave function with Fermi wave number at the origin.

This shows that for fixed $R_o$, the polarization at the

non-magnetic site oscillates with an extra phase $2\delta_o^F$, the phase shift $\delta_o^F$ being determined by the strength of the potential $V_o$.

More recently [6] , a formal study of the magnetic response to the local magnetic field associated to the exchange interaction between a two-band metal and a localized spin has been developed, including a spin-independent localized potential acting at the same site as the localized spin. A general expression was obtained in ref. [6] for the spin polarization induced by the spin (supposed in that case to be the magnetic rare earth spin moment) at an arbitrary site $R_j$ of the alloy.

In this paper we want to discuss in more detail the behavior at the impurity site of a two-band s-d electron gas with charge and spin perturbations lying at the same site. In this case a "genuine", well defined spin and a charge potential are introduced simultaneously by the impurity [6] . This study extends (to s-d transition metals) the previous works [4], where the spin and the charge potentials were located at next neighbours (corresponding to the limit $R_o = 0$ of ref. [4] ).

We investigate the behavior and sign of the contributions (s- and d-) to the total hyperfine field at the perturbed site, either for a fixed host as a function of band structure or as a function of the strength of the charge potential. The behavior as a function of band filling is obtained through screening arguments (see Sect. V).

In second place, we argue that this superposition at a same site of a charge and spin potentials is realized in practice whenever a rare earth impurity is dissolved in another metal, be it a 3d, 4d, 5d transition metal. Several experimental situations could be connected to this picture, e.g., rare-earth impurities in transition hosts as viewed from the hyperfine interactions, the possibility of studying spin glasses through hyperfine field measurements, and so on.

The situation provided by rare earth impurities diluted in s-p and noble metals can be handled in a similar way (Anderson-Moriya like approach) [7,8]. This is the subject of another work [9] .

Now, we give an outline of the paper. In Section II, we present the adopted model. In Section III we exhibit formal results for the s- and d- contributions for the hyperfine field,

whereas Section IV is devoted to the numerical analysis of the local magnetic responses.

In Section V, using the results obtained in the previous sections, and taking explicitly into account the self-consistent determination of the impurity potential matrix elements through Friedel sum rule [10], we discuss the hyperfine field at the impurity center. In Section VI, we summarize the main results discussed throughout this work, we discuss available experimental data and we suggest further experiments.

## II. THE MODEL

We consider the case of a magnetic rare-earth impurity placed in a transition metal like host [6].

The pure metal is described by two s- and d- non-hybridized bands, through

$$H_o = \sum_{ij\sigma} T_{ij}^{(s)} \; c_{i\sigma}^{+} \, c_{j\sigma} + \sum_{ij\sigma} T_{ij}^{(d)} \; d_{i\sigma}^{+} \, d_{j\sigma} \qquad (2.1)$$

(we refer the reader to refs. [6,11] for notation and definition of the terms).

Effects concerning d-band degeneracy (e.g., considering the partial density of states $\rho(\omega, \Gamma_{25}')$ and $\rho(\omega,\Gamma_{12})$ for cubic metals), are taken into account in a simplified way, using five identical d-subbands.

Besides the usual exchange coupling of the impurity with the conduction electron gas, given by

$$H_{exch}^{imp} = - \sum_{\sigma} \sigma \langle S^z \rangle \{ J^{(s)} c_{o\sigma}^{+} \, c_{o\sigma} + J^{(d)} \, d_{o\sigma}^{+} \, d_{o\sigma} \} \; , \qquad (2.2)$$

we take into account the spin independent charge potential, which is assumed to act only at the origin,

$$H_{ch}^{imp} = \sum_{\sigma} V_{dd}\, d_{o\sigma}^{+} d_{o\sigma} + \sum_{\sigma} (V_{sd}\, c_{o\sigma}^{+}\, d_{o\sigma} + V_{ds}\, d_{o\sigma}^{+}\, c_{o\sigma}) \qquad (2.3)$$

We completely neglect s-s intraband scattering. Moreover, the impurity induced d-d scattering may be determined, assuming that screening is entirely performed within the d-band, whereas the impurity induced mixing matrix element $V_{sd}$ is considered in this work as a phenomenological parameter (see below), its role being only to provide a channel of scattering for s-electrons.

The hamiltonian (2.3) plays an important role in the description of such strongly perturbed systems, since a large charge difference exists between the usually trivalent rare earth impurity and the transition metals (e.g., 0.5 holes in the Palladium d-band host).

Rare earth 5d states are quite different from m-d (m = = 3,4,5) states of usual transition or noble metals or inter - metallics. One expects, in general, two kind of new effects, namely: period effects [12] and variation of the Coulomb interaction at the impurity site [6].

Period effects are partially included in the self-consistent determination of $V_{dd}$, considering different bandwidths. A more complete treatment may be performed using the techniques due to Demangeat and Gautier [12].

The main effect of the Coulomb correlation at the impurity site is to "enhance" the local magnetic responses by a Stoner-like "enhancement" field [6]. This contribution is for the non degenerate case:

$$H_{Coul}^{imp} = \Delta U\, n_{o\uparrow}^{(d)}\; n_{o\downarrow}^{(d)} \;;\quad \Delta U = U_{imp} - U_{host}\,, \qquad (2.4)$$

U being the Coulomb repulsion parameter. For 5d impurities in 3d ir 4d hosts, $\Delta U$ is negative. For simplicity sake [13], we neglect Coulomb correlations in the host metal ($H_o$ term). If degeneracy is taken into account, one should incorporate contri-

butions from both exchange and Coulomb repulsion (see Sect. V).

So the adopted model hamiltonian for magnetic rare earth embedded in a transition metal-like host is

$$H = H_o + H_{ch}^{imp} + H_{exch}^{imp} + H_{Coul}^{imp} \qquad (2.5)$$

## III. SELF POLARIZATION HYPERFINE FIELD: FORMAL RESULTS

In this Section we establish expressions which enable us to discuss specifically the self-polarization hyperfine field induced by the rare earth's f-spin.

The impurity rare-earth magnetic moment produces a local field, which polarizes the conduction states, thus creating, via the contact and core polarizations a hyperfine field on its own nucleus. No orbital effects are included in this work; in particular, the rare-earth's magnetic moment is assumed to arise entirely from the spin moment (s-state ions).

Using expressions 18 from ref. 6, summing up over q, one gets for the s- and d- parts of the self polarization field,

$$H_{hf}^{(s)} = 2A(Z)J^{(s)} \langle S^z \rangle \cdot \chi_{free}^{ss}(0) \left\{ 1 + 2 \frac{\delta \bar{\chi}^{ss}(0)}{\chi_{free}^{ss}(0)} + \right.$$

$$\left. + \frac{J^{(d)}}{J^{(s)}} \frac{\bar{\chi}^{mix}(0)}{\chi_{free}^{ss}(0)} \right\} , \qquad (3.1)$$

$$H_{hf}^{(d)} = -2A_{cp} J^{(d)} \langle S^z \rangle \chi^{dd}(0) \left\{ 1 + \frac{J^{(s)}}{J^{(d)}} \frac{\bar{\chi}^{mix}(0)}{\bar{\chi}^{dd}(0)} \right\}, \qquad (3.2)$$

where $A(Z)$ and $A_{cp} > 0$ are the contact and core polarization coupling constants, estimated for several cases |1|, whereas $\langle S^z \rangle$ , $J^{(\lambda)}$, ($\lambda$=s,d) are the average z- component of the impurity rare earth spin and the exchange couplings respectively.

Now, we quote the expressions (at T = 0°K) for the static local magnetic responses which appear in the above equations.

(i) The s-s local magnetic response in the absence of potential scattering, $\chi^{ss}_{free}(0)$ is given by

$$\chi^{ss}_{free}(0) = -2\int_{E_b}^{\epsilon_F} F_s^R(\omega)\rho_s(\omega)d\omega = \frac{1}{\pi}\,\mathrm{Im}\int_{E_b}^{\epsilon_F} |F_s(\omega)|^2 d\omega$$

$$= \int_{E_b}^{\epsilon_F} |F_s(\omega)|^2 \sin[2\delta_s(\omega)]\, d\omega, \qquad (3.3a)$$

where $E_b$ is the bottom of the band.

So, $\chi^{ss}_{free}(0)$ is completely specified by the s-like part of the band structure.

(ii) The complete d-d local magnetic susceptibility $\chi^{dd}(0)$ is calculated in detail in ref. 6. At T = 0°K, one has for the local response in the absence of Coulomb interactions,

$$\chi^{dd}(0) = \frac{5}{\pi}\int_{E_b}^{\epsilon_F} \frac{|F_d(\omega)|^2}{|X(\omega)|^2} \sin[2\eta(\omega) - 2\delta_d(\omega)]d\omega \qquad (3.3b)$$

The presence of Coulomb interactions implies [6]

$$\chi^{dd}(0) = \frac{\chi^{dd}(0)}{1-\Delta U\chi^{dd}(0)} \qquad (3.3c)$$

(iii) The change in s-s local magnetic susceptibility, due to impurity potential effects (transferred through impurity induced

s-d hybridizations), is

$$\delta\bar{\chi}^{ss}(0) = \delta\chi^{ss}(0)/(1-\Delta U\ \chi^{dd}(0)) \qquad (3.3d)$$

where

$$\delta\chi^{ss}(0) = \frac{5}{\pi}\left|V_{sd}\right|^2 \int_{E_b}^{\epsilon_F} \frac{|F_s(\omega)|^3|F_d(\omega)|}{|\chi(\omega)|} \sin[\eta(\omega)-3\delta_s(\omega)-\delta_d(\omega)]\,d\omega \qquad (3.3e)$$

(iv) The "cross" local magnetic susceptibility is given by

$$\bar{\chi}^{mix}(0) = \bar{\chi}^{sd}(0) = \bar{\chi}^{ds}(0) = \chi^{mix}(0)/(1 - \Delta U\ \chi^{dd}(0)) \qquad (3.3f)$$

where

$$\chi^{(mix)}(0) = \chi^{sd}(0) = \chi^{ds}(0) = \frac{5}{\pi}\left|V_{sd}\right|^2 \int_{E_b}^{\epsilon_F} \frac{|F_s(\omega)|^2|F_d(\omega)|^2}{|\chi(\omega)|^2} \times$$

$$\times \sin\left[2\eta(\omega) - 2\delta_s(\omega) - 2\delta_d(\omega)\right] d\omega\,. \qquad (3.3g)$$

The factor 5 in the above formulae accounts for the d-band degeneracy in our simplified description of degenerate bands, $\Delta U$ being accordingly replaced by $\Delta U = \Delta U + 4\Delta J$, where $\Delta J$ is the change in the local exchange interaction. For the definitions of the phase-shifts $\delta_\lambda(\omega)$ and $\eta(\omega)$ and the functions $|F_\lambda(\omega)|$ and $|\chi(\omega)|$ we refer the reader to references 6 and 11.

For vanishing impurity potential, the local magnetic susceptibilities $\bar{\delta\chi}^{ss}(0)$ and $\bar{\chi}^{mix}(0)$, which are proportional to $|V_{sd}|^2$ should vanish, whereas the local d-d magnetic response $\chi^{dd}(0)$ reduces to

$$\chi^{dd}_{free}(0) = -2\int_{E_b}^{\epsilon_F} F^R_d(\omega)\rho_d(\omega)d\omega = \frac{1}{\pi}\,\mathrm{Im}\int_{E_b}^{\epsilon_F} |F_d(\omega)|^2 d\omega, \qquad (3.6)$$

which is formally equal to (3.3a).

At this point, we summarize the main assumptions on which this work is based.

(i) We assume that screening is entirely performed within the d-band (high density of states at the Fermi level), satisfying Friedel's sum rule [10]

$$\Delta Z = -\frac{10}{\pi}\,\mathrm{arc\ tg}\,\frac{\pi V_{dd}\rho_d(\epsilon_F)}{1 - V_{dd}F^R_d(\epsilon_F)}, \qquad (3.7)$$

where $\Delta Z$ is the extra charge introduced by the impurity, $\epsilon_F$ is the Fermi level, and the factor 10 accounts for spin and orbital degeneracy for our non-magnetic hosts. So coherently neglect $|V_{sd}|^2$ corrections in the functions $X(\omega)$ appearing in the local magnetic responses, namely

$$|X(\omega)| = |X_{dd}(\omega)| = \{[1 - V_{dd}F^R_d(\omega)]^2 + [\pi V_{dd}\rho_d(\omega)]^2\}^{\frac{1}{2}}$$

Using (3.7) for the determination of $V_{dd}$ throughout this paper, we simplify the general expression for $V_{dd}$ obtained in eqns. (27) and (28) of ref. 6. That paper includes the role of $\Delta U$ in the charge screening condition. We expect that such simplification is not crucial to our final results. Physically, this approximation corresponds to neglect the scattering induced by $\Delta U$ in the perturbed one-electron propagators used to compute the local magnetic responses $\bar{\chi}^{\lambda\mu}(0)$. So, the only retained effect due to $\Delta U$ in the present work is to locally "enhance" the quantities $\chi^{dd}(0)$, $\chi^{mix}(0)$, $\delta\chi^{ss}(0)$ by a factor $[1 - \Delta U\,\chi^{dd}(0)]^{-1}$.

(ii) $V_{sd}$ is taken as a phenomenological parameter, (which will be approximately related to $V_{dd}$ later on): its role is to act only as a source of scattering between s and d states; it is the unique source of scattering for the s-electrons. $|V_{sd}|^2$ goes to zero with vanishing impurity potential.

One can account for the s-d "cross" effects in the screening, from first principles, following the procedure due to Riedinger and Gautier [14]. However, our oversimplified picture provides simple expressions for the self-polarization field, which can be easily evaluated numerically. In fact, the contributions $H_{hf}^{(\lambda)}$, ($\lambda$= s,d) are given in terms of local magnetic responses, which envolve, basically, the $\lambda$-densities of states and the respective Hilbert transforms.

## IV. NUMERICAL RESULTS

### A. Model for the host

Now, we present some numerical calculations to illustrate the theoretical results obtained in the preceding Section.

(i) We take "parabolic bands", chosen as

$$\rho_\lambda(\omega) = \alpha_\lambda \, (\omega^2 - \Delta_\lambda^2), \ (\lambda = s \text{ or } d), \qquad (4.1)$$

where the $\alpha_\lambda$ are normalization constants, which are taken as $0.75\ \Delta_\lambda^{-1}$ in order to give 1 electron per atom (degeneracy is included in the above formulae) and $\Delta_\lambda$ are the $\lambda$-band widths ($\lambda$= s or d). The values of $\Delta_\lambda$ are chosen through usual estimates from band calculations, (e.g., $\Delta_d/\Delta_s$ between 0.2 and 0.4, for transition metals).

(ii) To bring out the effects due to the changes d-band shape in transition metals, we take a "triangular" density of states model for the d-band given by

$$\rho_d(\omega) = \begin{cases} 0.3\omega + 0.3 & , \quad -1 \leq \omega \leq 0.4 \\ 5.67\omega - 1.84 & , \quad 0.4 \leq \omega \leq 0.7 \\ -7.09\omega + 7.09 & , \quad 0.7 \leq \omega \leq 1 \end{cases} . \qquad (4.2)$$

B. Description of the local magnetic responses

Figure 1 shows plots of the d-d local susceptibility $\chi^{dd}(0 ; V_{dd})$ as a function of the Fermi energy $\varepsilon_F$, for the model density of states defined in (4.1).

As an illustration, we exhibit the plot of the susceptibility $\chi^{dd}_{free}(0) = \sum_q \chi^{dd}(q ; V_{dd} = 0)$ (see 3.6), together with the magnetic response to an uniform magnetic field, $\chi^{dd}(q=0 ; V_{dd}=0) = \chi^{dd}_{free}(q = 0)$, which is proportional to the d-density of states $\rho_d(\varepsilon_F)$. One observes for $\chi^{dd}_{free}(0)$, compared to $\chi^{dd}_{free}(q = 0)$ a rounding of the local susceptibility at the band edges and an increase in the middle of the band. These effects become more explicit in fig. 2, when the model for the d-density of states is defined by (4.2).

Let us consider now, the results for $\chi^{dd}(0 ; V_{dd} \neq 0)$, in both situations of figs. 1 and 2. One may distinguish two regimes.

(i) When the potentials $V_{dd}$ are such that $V_{dd} < V_{dd}^{crit}$, where $V_{dd}^{crit} = |F_d^R(E_t)|^{-1}$, ($E_t$ being the energy of the top of the d-band), is just the potential necessary to repel a bound state, one verifies a tendency toward "piling up" the susceptibility for values of Fermi energy $\varepsilon_F$ close to the top of the band. This tendency persists, as long as $V_{dd}$ is increasing no matter the specific shape of the adopted band structure. The critical value for the existence of bound states depends on the particular choice of the model band shape. For instance, $V_{dd}^{crit} = 0.667$ and $V_{dd}^{crit} = 0.295$ depending on whether one considers (4.1) or (4.2) for the d-density of states. One may describe the general behaviour of $\chi^{dd}(0 ; V_{dd})$ as follows. For values of the energy near the bottom of the d-band, the local magnetic response is smaller than the cor

responding one in the absence of impurity scattering. This suggests a decrease in the number of states available to be polarized. For a certain energy $E_I(V_{dd})$, (which depends on the value of $V_{dd}$), one has $\chi^{dd}(0; V_{dd} \neq 0) = \chi^{dd}_{free}(0)$. For $\varepsilon_F > E_I$, one always has $\chi^{dd}(0; V_{dd} \neq 0) > \chi^{dd}_{free}(0)$. The general behaviour of $\chi^{dd}(0; V_{dd} \neq 0)$, for $\varepsilon_F > E_I$ is an initial increase up to its maximum value, then a rapid drop to zero, at the top of the band. This behaviour may be followed numerically plotting the function

$$g(\omega) = \frac{|F_d(\omega)|^2}{|\chi(\omega)|^2} \sin \; 2\eta_{dd}(\omega) - 2\delta_d(\omega) \quad ,$$

which is simply the derivative of $\chi^{dd}(0 ; V_{dd})$ with respect to $\varepsilon_F$, $V_{dd}$ being kept constant. At the top of the band, $\chi^{dd}(0; V_{dd})$ tends to zero with negative slope (i.e., $\frac{\partial}{\partial \varepsilon_F} \chi^{dd}(0;V_{dd}) < 0$). This follows remembering that $\eta_{dd}(\omega)$ goes to zero as $\omega$ goes to $E_t$ and $\delta_d(E_t) = -\pi$, and therefore the argument of the sine is close to $2\pi$. So, the localization of the maximum value of $\chi^{dd}(0;V_{dd})$ may be easily obtained accurately, through the change of sign of $\frac{\partial}{\partial \varepsilon_F} \chi^{dd}(0;V_{dd})$ from positive to negative values.

(ii) After a bound state is repelled, (i.e., $V_{dd} > V_{dd}^{crit}$), $\chi^{dd}(0;V_{dd})$ saturates. This general behaviour may be easily understood by considering the function $g(\omega) = \frac{\partial}{\partial \varepsilon_F} \chi^{dd}(0;V_{dd})$. In fact, if $V_{dd} > V_{dd}^{crit}$, $[2\eta_{dd}(\omega) - 2\delta_d(\omega)]^F$ is very small at the top of the band (see figs. 3 and 4), so that $\sin [2\eta_{dd}(\omega) - 2\delta_d(\omega)]$ is positive there. This contrasts with the $V < V_{crit}$ regime, where $2\eta_{dd}(E_t) - 2\delta_d(E_t) \simeq 2\pi$. In these conditions, the rapid drop of $\chi^{dd}(0;V_{dd})$ near the top of the band which is observed for $V_{dd} < V_{dd}^{crit}$ disappears, and $\chi^{dd}(0;V_{dd})$ saturates. One can understand such a behaviour, with the following hand waving argument. The extracted bound state is built up from band states spread out over the entire band. Comparing in fig. 1 the curves corresponding to $V_{dd} = 0.6$ (no bound state) and $V_{dd} = 0.8$ (bound state extracted), one sees that a certain amount of available states to be magnetized at the origin were used to built up the amplitude at the origin of the

empty bound state. So, the maximum value of $\chi^{dd}(0; V_{dd})$ is associated to the top of the band, since one obtains there the maximum contribution from the remaining band states to be polarized at the origin. Note that, for increasing $V_{dd}$, the amplitude of the bound state at the origin tends to 1, thus completely emptying the band states. From this numerical study one verifies that contrary to previously expected [6] no change in sign of $\chi^{dd}(0)$ occurs. Now, some comments about the quantities $\delta\chi^{ss}(0)$ and $\chi^{mix}(0)$. The ratio $\delta\chi^{ss}(0)/\chi^{ss}_{free}(0)$ turns out to be very small as compared to $\chi^{mix}(0)/\chi^{ss}_{free}(0)$. This is because $\delta\chi^{ss}(0)$ is associated with a scattering involving d-states only as intermediate states, the initial and final states being s-like. In view of that, we neglect the term $\delta\chi^{ss}(0)/\chi^{ss}_{free}(0)$ in our numerical estimates of the corrections to the "bare" s-hyperfine field.

Therefore, the adopted expression for the total s-like contribution to the hyperfine field is (cf. 3.1)

$$H^{(s)}_{hf} = 2A(Z) \langle S^z \rangle J^{(s)} \chi^{ss}_{free}(0)\{1 + \frac{J^{(d)}}{J^{(s)}} \frac{\chi^{mix}(0)}{\chi^{ss}_{free}(0)}\} \qquad (4.3)$$

If for reasonable values of the exchange interactions $J^{(s)}$, $J^{(d)}$ ($J^{(d)}/J^{(s)} \simeq 2$ [15] ), the s-part of the hyperfine field is to change sign, such a behaviour is connected to a possible change in sign of the "cross" magnetic response $\chi^{mix}(0)$, since $\chi^{ss}_{free}(0)$ is essentially positive.

Recall that (3.3g ) should be compared to (3.3b) and (3.3a). In those expressions one, has respectively $\sin[2\eta(\omega)-2\delta_d(\omega)]$ and $\sin[2\delta_s(\omega)]$. The simultaneous existence of the arguments $2\eta(\omega) - 2\delta_d(\omega)$ and $2\delta_s(\omega)$ in (3.3g) just reflects the physical processes involved, which give rise to $\chi^{mix}(0)$. In fact, one looks for e.g. the s-response to the local d-exchange field. This involves simultaneously the s-propagators and the impurity perturbed d-propagator, the transition between s- and d-states being ensured by the impurity induced s-d mixing.

We have discussed numerically the influence of the various

relevant parameters for the change in sign of $\chi^{mix}(0)$ as a function of $\varepsilon_F$. As far as changes of sign are concerned and within the approximation that screening is only performed by d-electrons, the values of $|V_{sd}|^2$ only affect the magnitude of $\chi^{mix}(0)$. (See below for an estimate of $|V_{sd}|^2$).

We conclude that the relevant parameters inducing a change in sign of $\chi^{mix}(0)$ are:

(i) The strength of the $V_{dd}$ potential;

(ii) The "phase shift" $\delta_s(\omega) = \text{arctg} \dfrac{\pi \rho_s(\omega)}{F_R^s(\omega)}$ which appears in the definition (3.4).

In fig. 5 we show, for the same values of $V_{dd}$, the influence of including the "phase shift" $\delta_s(\omega)$ possible change- in sign for $\chi^{mix}(0)$. One can see that change in sign can be supressed if the term $\delta_s(\omega)$, which is connected to the unperturbed s-band, is disregarded.

The "enhancement" effects, not included in the numerical results discussed in this paragraph only reduce (for negative $\Delta U$) the values obtained for $\chi^{dd}(0)$ and $\chi^{mix}(0)$. In the self-consistent calculations, exhibited in the next section, this effect is explicity included. Anyhow, the considerations about piling up of states and changes in sign, discussed above, are not destroyed by the inclusion of $\Delta U$, only orders of magnitude being involved.

## V. SELF CONSISTENT RESULTS

In the preceding Section we have discussed numerically the behaviour of the local susceptibilities $\chi^{\lambda\mu}(0)$, $(\lambda,\mu = s,d)$ as a function of several possible values for the Fermi energy $\varepsilon_F$ and for several values of the matrix elements $V_{dd}$. In that Section $|V_{sd}|^2$ was taken constant and we have illustrated the result for $\chi^{mix}(0)$, taking $|V_{sd}|^2 = 0.8$ (see below).

This Section is devoted to calculate the hyperfine field in real situations, namely with the band filling corresponding to several metals in the Periodic Table.

Before entering in the details of the numerical results, we briefly recall the essentials of the hyperfine field of dilute rare earth impurities in transition metals. The total hyperfine field associated to the rare earth (small concentration of impurities) is a sum of three terms:

(i) The f core state hyperfine field, assumed to be known from experiments in insulating materials;

(ii) The self-polarization hyperfine field, which we estimate in the present work;

(iii) The transferred field, which is not computed here. An experimental estimate of this last contribution can be obtained using small quantities of Lutetium impurities (no spin moment) together with spin carrying rare earths (e.g., $(Lu_xGd_{1-x})_y\ T_{1-y}$), T being a transition metal host, and $x,y << 1$).

In the light of previous works [1,4], we have reduced our formal results to ratios as far as hyperfine constants are concerned. In fact, we express the rare earth self polarization field in units of $J^{(s)}A(Z)\langle S^z\rangle$ and the remaining dependance on $A_{cp}$ and $A(Z)$ appears through the ratio $A_{cp}/A(Z)$. From eqns. (4.3) and (3.2) one gets

$$\frac{H_{\perp}^{total}}{J^{(s)}} \frac{A_{cp}}{A(Z)} \bar{\chi}^{dd}_{corrected}(0) \quad , \tag{5.1}$$

$$\left. \frac{\bar{\chi}^{mix}(0)}{\chi^{ss}_{free}(0)} \right\} \quad , \tag{5.2a}$$

$$\left. \frac{\bar{\chi}^{mix}(0)}{\chi^{dd}(0)} \right\} \quad . \tag{5.2b}$$

Once we consider rare earths (5d states) we use Campbell's [1] estimate of $A_{cp}$ for 5d elements and A(Z) appropriate to rare earths. Since s-d hybridization is incorporated in Ref. 1 in a quite subtle way we hope that taking the ratio $A_{cp}/A(Z)$ one gets simultaneously consistency with the spirit of that calculation [1] and a flexible parameter to adjust when experimental data is available.

Now, a few comments about the sign of the exchange couplings $J^{(\lambda)}$, ($\lambda$ = s or d). Usually the d-f exchange interaction $J^{(d)}$ is taken as a positive quantity. However, recent experimental results concerning ESR experiments in bottlenecked systems suggest the possibility of negative exchange coupling, the origin of such a coupling being ascribed to a direct d-f Heisenberg like exchange between next neighbour d and f orbitals [16]. We will investigate later on the influence of the sign of $J^{(d)}$ in the self-polarization field. Such a study may provide an experimental check of the model proposed by Rettori et al. [16] for ESR results through self-polarization hyperfine field measurements.

In what follows, we sketch the program of the numerical estimates of this Section. Using the approximate screening condition (3.7) where $\Delta U$ corrections are neglected and once the Fermi level is fixed by the host band filling $n_e$, one obtains self consistently the $V_{dd}$ matrix element suitable to screen the charge difference $\Delta Z = 3-n_e$.

We take [17]

$$|V_{sd}|^2 = v_{sd}^2 \; |V_{dd}|^2 \; ; \; v_{sd} = \frac{\langle s|v|d\rangle}{\langle d|v|d\rangle} \; , \tag{5.3}$$

v being the impurity potential form factor. This is consistent with the Friedel sum rule estimative of $V_{dd}$. So, we have transferred the phenomenological character of $|V_{sd}|^2$ to the potential form factor $v_{sd}$. Therefore, once the factor $v_{sd}$ is given or estimated, the potential matrix elements are completely specified.

We discuss here the role of bandwidths (s- and d-), hybridization form factor, sign of the ratio of exchange couplings and the effect of the local "exchange enhancement" due to $\Delta U$ in the self polarization field.

The Moriya-like density of states defined by (4.1) for the s- and d- bands is used to simulate for band fillings ranging from $n_e = 5$ electrons to $n_e = 9$ electrons, the role of different bandwidths (or ratio of bandwidths).

In order to get a feeling for a more realistic d-band structure, we also present results obtained using the "triangular" model density of states defined by (4.2). Clearly a realistic band structure density of states can be used as an entry data in our calculation, since the expressions for the local responses $\chi^{\lambda\mu}(0)$, $(\lambda,\mu = s,d)$, depend on the host density of states $\rho_\lambda(\omega)$, its Hilbert transform $F_\lambda^R(\omega)$ and the impurity charge difference.

In figure 6 we show the total self polarization field as given by (5.1) for increasing d-bandwidths, the s-bandwidth being kept constant ($\Delta_d = 1$ and $5/3$; $\Delta_s = 5$). This situation simulates the d-bandwidth contribution to period effects (e.g. rare earths impurities in 4d and 5d metals) and may also crudely describe pressure effects. It turns out that the minimum value (maximum in absolute value) shifts from the middle of the series to the end of the series when one increases the d-bandwidth.

Concerning the sign of the exchange couplings two situations are shown: $J^{(d)} > 0$, $J^{(s)} > 0$ which corresponds to a negative hyperfine field and $J^{(d)} < 0$, $J^{(s)} > 0$ corresponding to a positive hyperfine field.

In figure 7 we illustrate the effect of the magnitude of the s-d hybridization form factor $v_{sd}$ in the total self-polarization field.

Together with the self-consistent results we show in figure 8 the d-like local magnetic response $\chi^{dd}(0;V_{dd})$ as a function of the Fermi energy $\varepsilon_F$, using the self-consistent values for $V_{dd}$ appropriate to the adopted band fillings. This figure in fact shows the construction of the d-like part of the hyperfine field, since the correction factor

$$\frac{J^{(s)}}{J^{(d)}} \frac{\bar{\chi}^{mix}(0)}{\bar{\chi}^{dd}(0)} = \frac{J^{(s)}}{J^{(d)}} \frac{\chi^{mix}(0)}{\chi^{dd}(0)}$$

is very small. So, the d-hyperfine contribution arises mainly

from the charge potential perturbed local d-d magnetic response $\chi^{dd}(0;V_{dd})$. The dotted curve exhibits the trend of the d-like hyperfine field.

The main features of the s-like contribution for the hyperfine field are showed in figure 9. One considers two possibilities for the sign of $J^{(d)}$, with $J^{(s)} > 0$. For the case of positive d-f exchange coupling one sees the possibility of a change in sign for the s-hyperfine field, which shows a close resemblance to the usual results for the s-p hyperfine fields in ferromagnetic alloys [1] . However, for negative d-f exchange coupling no change in sign is expected. In fact, change in sign is associated (see 5.2a) to competition between $\chi^{mix}(0)$ and $\chi^{ss}_{free}(0)$. So, for a given ratio $J^{(d)}/J^{(s)}$ and since $\chi^{mix}(0)$ is negative, no change in sign is expected for $H^{(s)}_{hf}$ if one takes $J^{(d)} < 0$. To illustrate this point we plot in this figure $\chi^{ss}_{free}(0)$ as a function of band filling $n_e$ . For a large s-band, $\chi^{ss}_{free}(0)$ is roughly constant in the region of interest). Expression (5.2a) implies a "symmetry" of the two curves with respect to $\chi^{ss}_{free}(0)$, which is indeed observed.

An essential result of our calculation which is to be contrasted with s-p impurities diluted in ferromagnetic alloys or in the case of Heusler alloys is the absence of change in sign in the total self-polarization field. Although the theoretical ingredients of the model are similar to that of Blandin and Campbell [4] , except for the limit $R_o \to 0$ implied by the nature of the rare earth impurity, the existence of a narrow and degenerate d-band which responds to the local magnetic field in a dominant way explains the difference between these cases.

Until now, in all results presented above we have disregarded the effect of $\Delta U$. Next, we investigate the role of local correlations in a strong "enhancement" case. This means $|\Delta U|$ of the order of 0.5 eV. In fact, we take into account, since degeneracy is present in our formulation, contributions from Coulomb and exchange interactions, i.e., $-0.5 = \Delta U + 4\Delta J = \Delta\tilde{U}$, where $\Delta J$ is the change in the local exchange interaction. We take $\Delta\tilde{U}$, since the 5d rare earths orbitals are expected to have larger extent than the 3d or 4d transition metal ones. For rare earths in 5d

metals one expects $\Delta\tilde{U} \simeq 0$; so the results including finite $\Delta\tilde{U}$ are expected to apply for rare earths in say 4d metals.

In figure 10 we illustrate this effect; we try to simulate a situation of a rare earth diluted in a 5d and in a 4d host. We expect a larger d-band width for the 5d than for a 4d host and also a stronger hybridization form factor for the 4d host. So, for the same s-band width one expects without "enhancement" a more pronounced effect in the 4d host than in the 5d one. In the 5d case, we take $\Delta\tilde{U} = 0$; thus keeping only one-electron effects. However, for the 4d case, we include $\Delta\tilde{U} = -0.5$. Figure 12 shows that concerning 4d hosts, expected dominant effects are wiped out and one obtains an almost constant total hyperfine field except a drop at the end of the 4d series. On the other hand, the 5d host exhibit a maximum when one passes from the middle to the end of the series. However, due to the small mixing form factor and large d-band width, the hyperfine values at the end and middle of the series are almost the same.

The peculiar behaviour of the local correlation effects can be understood in the following way. The "enhancement" correction appears in the s- and d- contributions correcting $\chi^{mix}(0)$ and $\chi^{dd}(0)$ by a factor $[1-\Delta U\chi^{dd}(0)]^{-1}$. As discussed above, the s-like part of the hyperfine field changes sign due to the term proportional to $\chi^{mix}(0)$. Since $\Delta U < 0$, one has $|\chi^{mix}(0)| < |\chi^{mix}(0)|$ and the s-like contribution becomes more slowly varying but still shows a change in sign. As far as the d-like part is concerned the effect of including the factor $[1-\Delta U\chi^{dd}(0)]^{-1}$ is much more pronounced: this factor drastically reduces the values of $\chi^{dd}(0)$ and grosso modo the d-hyperfine contribution turns out to be reduced to a half of the one electron only d-hyperfine field. These two features are clearly exhibited in figures 11 and 12.

Finally, in order to check the dependence of the trends discussed above on the model density of states we have also performed a self-consistent calculation using the triangular density of states defined by (4.2). We illustrate our results in figures 13, 2 and 14. The same general tendencies are conserved.

## VI. FINAL COMMENTS AND CONNECTION WITH EXPERIMENTAL SITUATION

A systematic study of the model description of magnetic rare earth impurities in transition metals has been developed throughout this paper. We emphasize the spirit of this calculation: starting from simple models for the density of states (defined by a few number of parameters), we systematically investigate the role of each parameter in the self-polarization hyperfine field. From this systematic numerical study it turns out that:

(i) The behaviour of the hyperfine field in this case contrasts strongly with the "changing sign" behaviour observed in s-p impurities in ferromagnetic alloys or Heusler alloys. Although the underlying physical mechanism of potential scattering plus exchange polarization is common to all these cases, the main difference in our work arises from the existence and importance of the unfilled narrow d-band. So we conclude that this last feature "screens" the effect of usual change in sign of the hyperfine field, its effect appearing only in the curvature of the hyperfine field as a function of band filling.

(ii) The role of increasing d-bandwidth, simulating period effects or applied pressure, manifests itself in shifting the maximum absolute value of the hyperfine field from the middle to the end of the transition metal series. The simulation of pressure effects through the increase of the d-bandwidth as compared to experimental results could be a good test for the impurity potential scattering approach of such effects.

(iii) The s-like part of the hyperfine field although not dominant in our case, still may show a change in sign as a function of the band filling. So, in the physical realization of the $R_o \to 0$ limit of Blandin and Campbell's work [4], the s-part contribution may change sign, the physical origin of this feature being ascribed to "cross" s-d-s scattering.

(iv) Our present calculation may provide a natural check of a possible connection between ESR experiments and hyperfine field interactions. In fact, as mentioned before in Sect. V, experimental

results obtained by Rettori et al. [16] on the ESR of rare earth impurities in several hosts exhibiting bottleneck effects suggest a negative value for the d-f exchange coupling $J^{(d)}$. Our results show that in such a situation the self-polarization hyperfine field is to be positive. So a systematic experimental study combining ESR experiments with hyperfine field measurements could be a good test for the theoretical model developed above.

Some experimental results are available at present; these involve transition metals and intermetallic compounds as hosts. ESR studies were performed for Er diluted in 4d and 5d hosts like Rh, Pd and Ir, Pt [18]. Defining the hyperfine constant $A_{eff}$ through $H_{hf} = A_{eff}\langle S^z\rangle/g_I u_I$, the experimental values of $A_{eff}$ for Er in these transition hosts lie between 75 and 77 gauss. This is to be compared with the value in insulators $A_{ins} = 71$ gauss. From these experiments one concludes that the value of the hyperfine constant id roughly the same for 4d or 5d hosts. Furthermore the effect of the metallic environment is to introduce a positive shift in the hyperfine constant, so $\Delta A = A_{eff} - A_{ins} > 0$ (orbital contributions are considered here as being untouched by the conduction gas).

Simultaneously g shift measurements indicate large and negative values consistent with the model suggested by Retorri et al. [16] for the nature and sign of the exchange couplings $J^{(d)}$.

These experimental results [16] are consistent with the theoretical picture presented throughout this work. In fact, since ESR g-shift is negative, the coupling $J^{(d)}$ is thought to be negative; also the total hyperfine field is predicted to be positive.

The almost identical hyperfine constants reported in refs. 18 fit also with our theoretical model. As discussed in Sect. V, one expects a smaller bandwidth for 4d hosts, consequently with larger d-d responses as compared to 5d ones. However, in 4d hosts, the presence of a local correlation parameter $\Delta\tilde{U}$ tends to reduce the hyperfine field (see figures 12 and 16). These competing mechanisms tend to compensate and give almost identical hyperfine fields. At this point we suggest further experimental studies involving 4d and 5d pure hosts to systematically analyse the above

mentioned period.effects in high d-density metals.

Concerning intermetallic compounds as hosts some experimental work is available [19] . Compounds like $ARh_2$ and $AIr_2$ (A = La, Y, Ce, Lu) doped with Gd or Nd show in the case of Nd, negative values for $\Delta A$. These compounds are thought to exhibit a small d-density of states (almost filled d-band) [19]. Since the g-shift turns out to be positive [19] again these results are consistent (for $J^{(d)} > 0$) with our theoretical model. Concerning the physical picture suggested in ref. 16 for the exchange coupling $J^{(d)}$, one expects a competition between intra-rare-earth site direct exchange (which is positive) and exchange with next-neighbour d-states (which is negative). So in a strong d-like metal, the screening condition amounts to reduce the direct intra-site exchange through the reduction of the occupation number of the rare earth site. Since the neighbour occupation is not to be changed appreciably, the negative contribution dominates. In these intermetallics ($ARh_2$, $AIr_2$), if the number of available d-conduction states of the neighbours of the rare earth are supposed to be small, even if d-states are present at the rare earth site the total coupling $J^{(d)}$ tends to be positive in agreement with experiment. These simple ideas can be used to evaluate numerically the exchange integral $J^{(d)}$ starting from impurity perturbed d-Bloch wave functions [20]. Using the simple model density of states (4.1) it turns out that a change in sign from positive to negative $J^{(d)}$ occurs around the middle of the n-d series. A more detailed account of this calculation will appear elsewhere [20].

Throughout this work $J^{(\lambda)}$, ($\lambda$= s,d) was assumed to be independent of k, k'. This is for simplicity reasons. If one conserves the full k, k' dependence one has to compute numerically the impurity perturbed magnetic responses $\chi^{\lambda\mu}(k,q)$, ($\lambda\mu$ = s,d). Such numerical computations involve complicated sums over the Brillouin zone since the susceptibilities $\chi^{\lambda\mu}(k,q)$ depend on the band dispersion relations $\varepsilon_k^{(\lambda)}$. This approximation should not invalidate the main results of this work since it amounts to taking an average value of the k, k' dependent exchange interaction, impurity effects being incorporated in the local magnetic responses $\chi^{\lambda\mu}(0)$ as given by (3.5).

Now a few comments on spin glasses. Until now the generalization of the Ruderman-Kittle-Kasuya-Yosida (RKKY) interaction to a strongly perturbed electron gas has been applied only to Heusler alloys [4] . In the formulation presented above it appears that the experimental situation of interest can be made more general than the cases mentioned previously [1-6]. In particular, the case of frozen spin disorder or spin glasses as a "new form" of magnetic order can be considered applying the ideas discussed throughout this work.

In view of that it would be interesting to have hyperfine field measurements in transition metal based-rare-earth spin glass systems. As mentioned before, the hyperfine field at a rare earth nucleus is the sum of the self-polarization field plus transferred hyperfine field. This last contribution includes all the statistics usually applied to describe spin glasses, with all the theoretical problems open. Then, we would suggest the following kind of experiment. Suppose a spin glass $R_xT_{1-x}$, (where R is a magnetic rare earth and T is the transition host) and the following one $(R_{1-y}Lu_y)\ T_{1-x}$, where we have replaced a very small quantity of magnetic rare earth (e.g., Gd) by a non magnetic one as Lu, and assuming that since Lu and Gd are both trivalent, only small changes on the spin glass behaviour occur. By separately measuring the hyperfine field at the Lutetium site [21] in the second spin glass sample and comparing to the hyperfine field measurement at the R site in the first spin glass sample, we hope that similarly to the case of ferromagnetic Gadolinium [21] we can separate those two contributions, namely transferred and self-polarization fields.

Due to the nature of the spin glass magnetic order, experimental difficulties concerning the orientation of the local magnetic moments may appear. The suggested hyperfine field experiments depend strongly on the experimental possibility of analyzing spectroscopic data. Recent experimental work shows that systems like $Gd_xTh_{1-x}\ Ru_2$ and $Gd_x\ Ce_{1-x}\ Ru_2$ exhibit spin glass behaviour [22]. These systems and those doped with Lu are natural candidates for the experimental study suggested above and the present work provides the theoretical tool needed to extract in-

formation on the spin glass order parameter from the knowledge of the self-polarization hyperfine field at the magnetic site, as derived from independent measurements at Gd and Lu sites.

The study of the temperature dependence of the order parameter of the spin glass phase [23] requires the extension in temperature of the computations presented here.

Acknowledgements

It is a pleasure to thank Professor D. Davidov for a very interesting and stimulating discussion. Two of us (A.T. and A.A.G.) gratefully acknowledge the members of the Laboratoire de Physique des Solides (Orsay) for their kind hospitality during 1976, where part of this work was performed.

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FIGURE CAPTIONS

Fig. 1 d-d local susceptibility $\chi^{dd}(0;V_{dd})$ for the band model (4.1) as a function of the Fermi energy for several values of the impurity matrix element $V_{dd}$.

Fig. 2 d-d local susceptibility $\chi^{dd}(0;V_{dd})$ evaluated for the "triangular" band model (4.2). The adopted $V_{dd}$ values are the self-consistent ones corresponding to band filling of 3 electrons to 9 electrons. The dotted line indicates the self-consistent values of $\chi^{dd}(0;V_{dd})$ for the band fillings.

Fig. 3 Phase shift $\eta_{dd}(\varepsilon_F)$ computed using the band model (4.1) for the same values of the potential $V_{dd}$ as in fig. 1.

Fig. 4 Phase shift $\eta_{dd}(\varepsilon_F)$ computed using the band model (4.2) for several self-consistent values of the $V_{dd}$ impurity potential.

Fig. 5 Cross susceptibility $\chi^{mix}(0)$ as a function of the Fermi energy $\varepsilon_F$ and impurity potential $V_{dd}$, for two cases: including the "phase-shift" $\delta_s(\varepsilon_F)$ (possibility of a change in sign of $\chi^{mix}(0)$ and neglecting $\delta_s(\varepsilon_F)$ ($\chi^{mix}(0) \geq 0$).

Fig. 6 Total hyperfine field (in units of $J^{(s)}A(Z)\langle S^z\rangle$) as a function of band filling (5 electrons to 9 electrons) for two different d- bandwidths. The s- bandwidth is kept constant.

Fig. 7 Total hyperfine field (in units of $J^{(s)}A(Z)\langle S^z\rangle$) as a function of the strength of the $v_{sd}$ hybridization form factor.

Fig. 8 d-d local susceptibility as a function of $\varepsilon_F$ for the self-consistent values of $V_{dd}$ corresponding to band fillings 5 to 9 for the band model (4.1).
The broken line gives the self-consistent values of $\chi^{dd}(0)$ corresponding to the band fillings.

Fig. 9 s-like contributions to the total hyperfine field (in units of $J^{(s)}A(Z)\langle S^z\rangle$) as a function of the coupling $J^{(d)}$ (positive and negative d-f couplings). For reference we plot the values of $\chi^{ss}_{free}(0)$.

Fig. 10 Effect of the local "enhancement" correction $\Delta\tilde{U}$ (see text).

Fig. 11 Effect of the local "enhancement" correction $\Delta\tilde{U}$ in the s-part (through $\overline{\chi}^{mix}(0)$ showing the persistence of a change in sign.

Fig. 12 Effect of the local "enhancement" correction $\Delta\tilde{U}$ in the d-part of the hyperfine field.

Fig. 13 s- and d- like contributions to the total hyperfine field (in units of $J^{(s)}A(Z)\langle S^z\rangle$) for the triangular band model (4.2) for band fillings ranging from 3 electrons to 9 electrons.

Fig. 14 Effect of the local "enhancement" correction $\Delta\tilde{U}$ for the band model defined by (4.2).

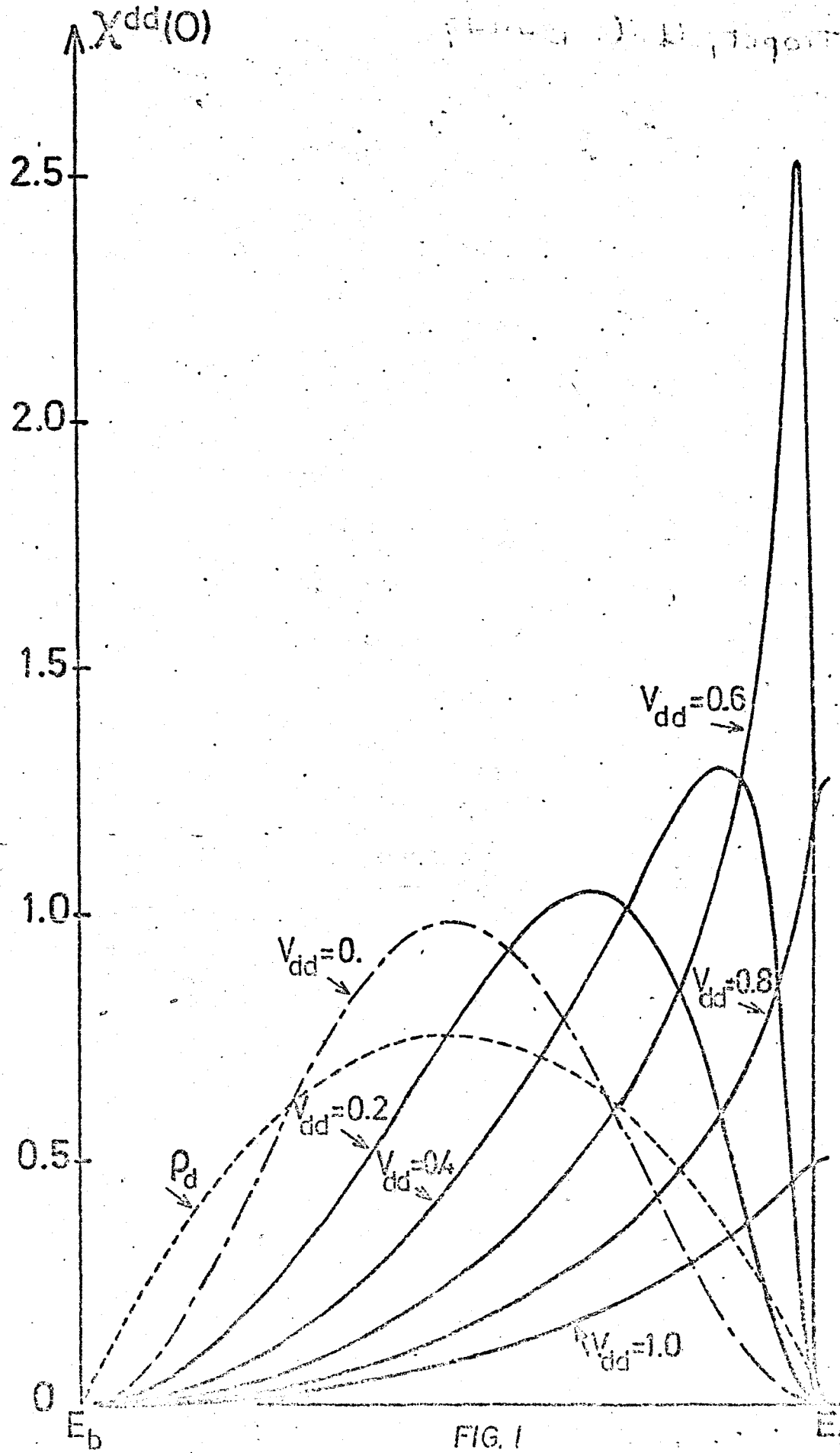
$\chi^{dd}(0)$
2.5
2.0
1.5
1.0
0.5
0
$V_{dd}$=0.6
$V_{dd}$=0.
$V_{dd}$=0.8
$V_{dd}$=0.2
$V_{dd}$=0.4
$\rho_d$
$V_{dd}$=1.0
$E_b$
$E_t$

FIG. 1

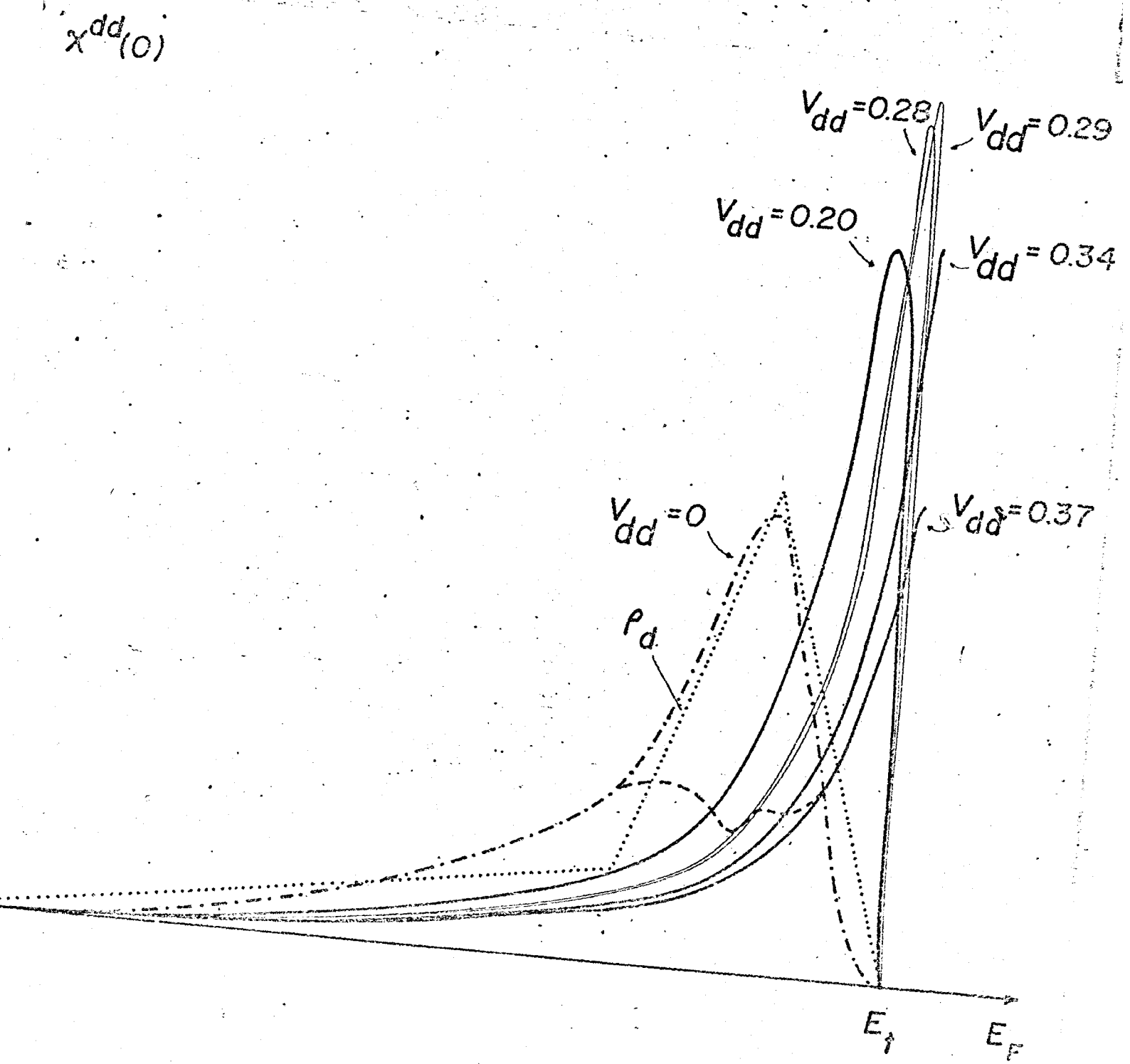
$\chi^{dd}(0)$
$V_{dd}=0.28$
$V_{dd}=0.29$
$V_{dd}=0.20$
$V_{dd}=0.34$
$V_{dd}=0$
$V_{dd}=0.37$
$\rho_d$
$E_\uparrow$
$E_F$

FIG. 2

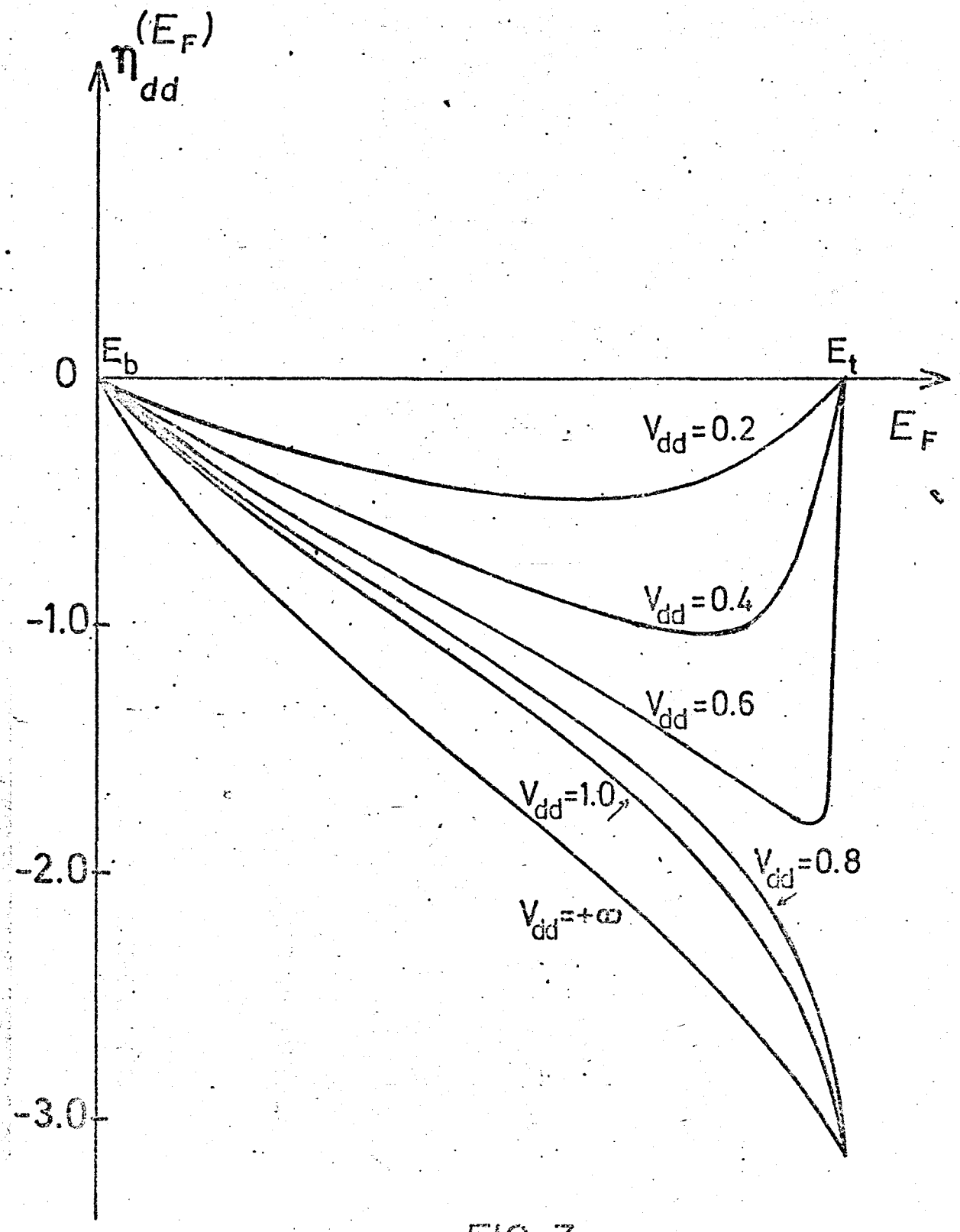
$\eta_{dd}^{(E_F)}$
0
$E_b$
$E_t$
$E_F$
-1.0
-2.0
-3.0
$V_{dd}=0.2$
$V_{dd}=0.4$
$V_{dd}=0.6$
$V_{dd}=0.8$
$V_{dd}=1.0$
$V_{dd}=+\infty$

FIG. 3

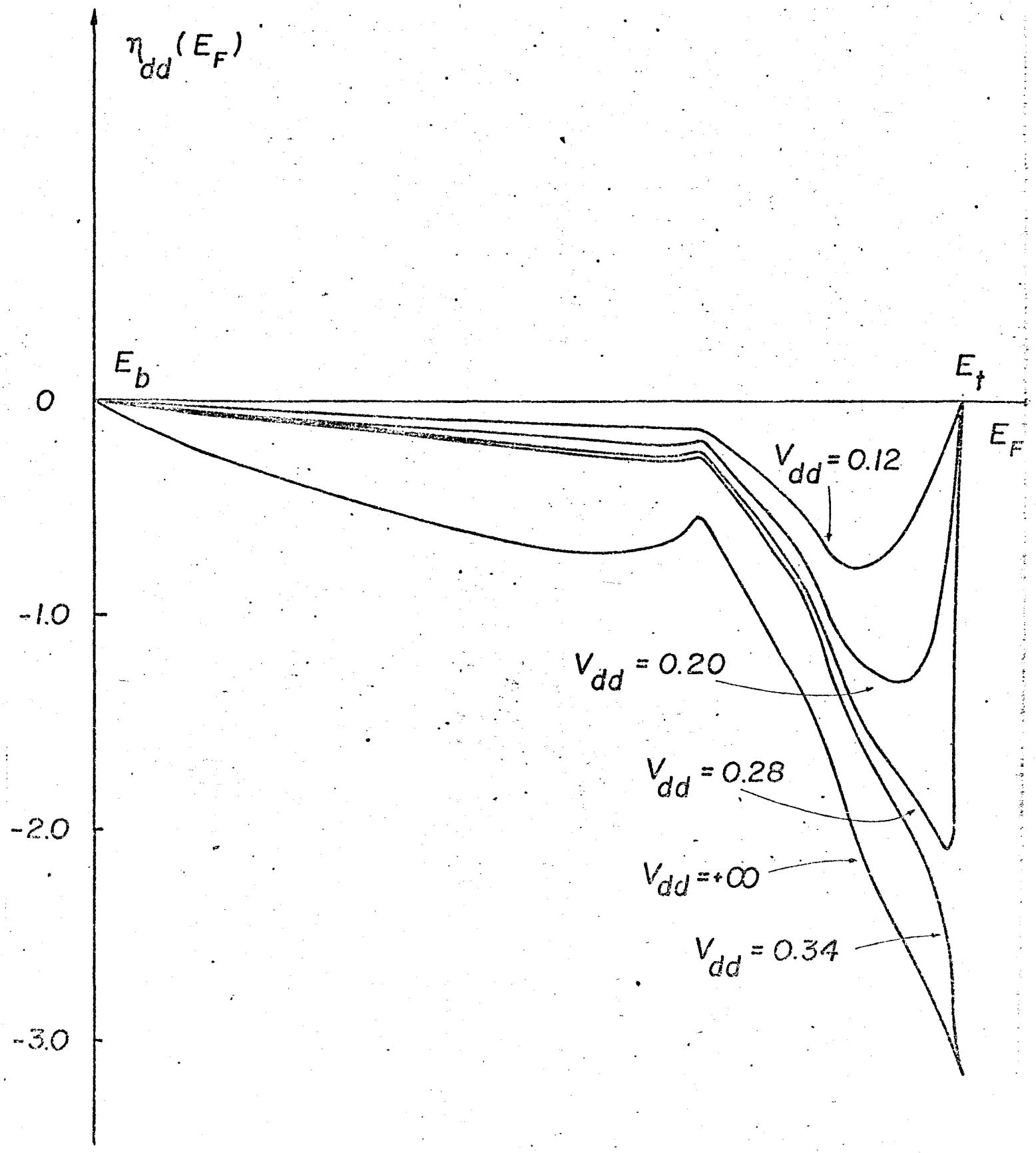
$\eta_{dd}(E_F)$
$E_b$
$E_t$
$E_F$
0
-1.0
-2.0
-3.0
$V_{dd} = 0.12$
$V_{dd} = 0.20$
$V_{dd} = 0.28$
$V_{dd} = +\infty$
$V_{dd} = 0.34$

FIG. 4

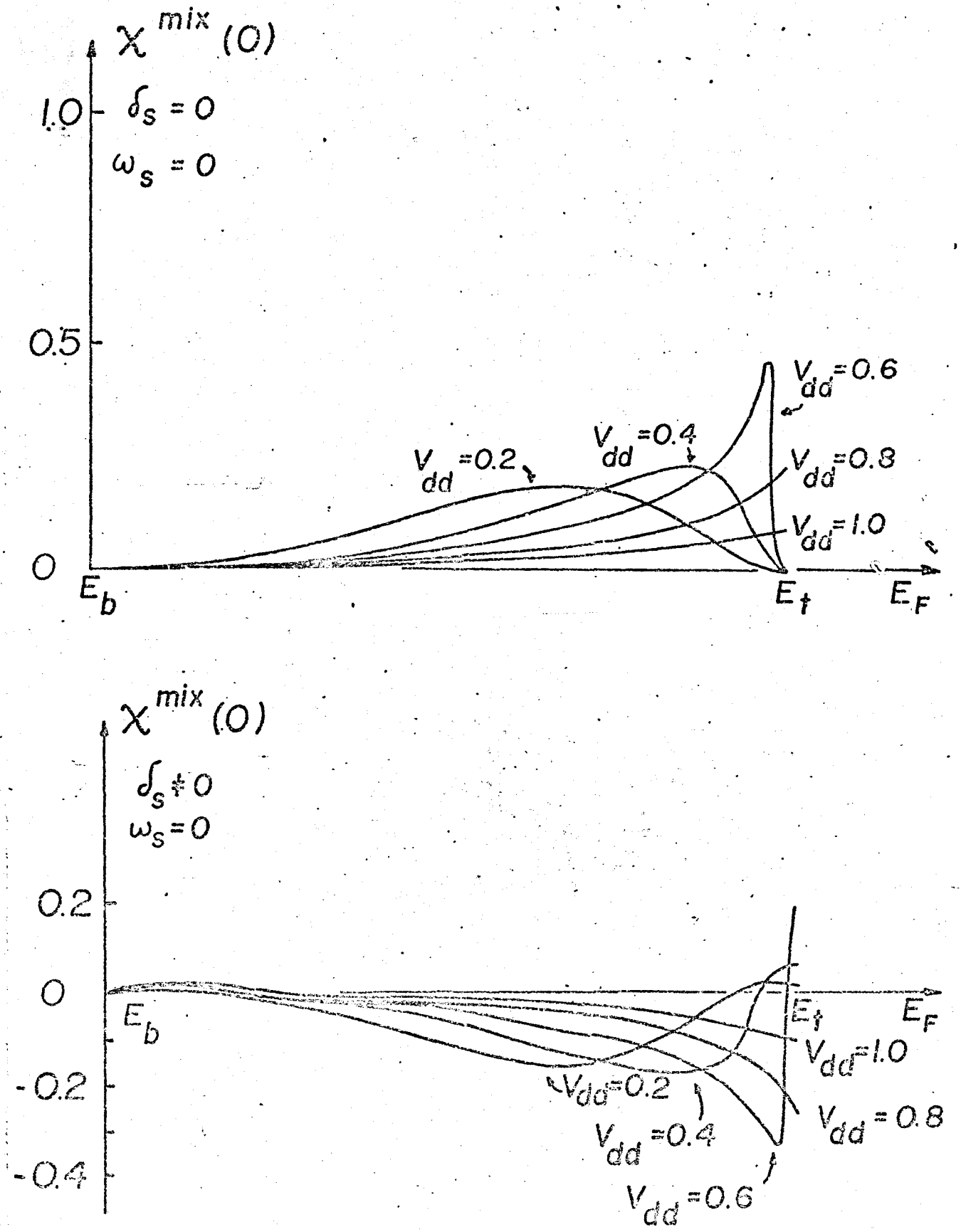
$\chi^{mix}(0)$
1.0
$\delta_s = 0$
$\omega_s = 0$
0.5
0
$E_b$
$E_t$
$E_F$
$V_{dd}=0.2$
$V_{dd}=0.4$
$V_{dd}=0.6$
$V_{dd}=0.8$
$V_{dd}=1.0$
$\chi^{mix}(0)$
$\delta_s \neq 0$
$\omega_s = 0$
0.2
0
-0.2
-0.4
$E_b$
$E_t$
$E_F$
$V_{dd}=1.0$
$V_{dd}=0.2$
$V_{dd}=0.4$
$V_{dd}=0.8$
$V_{dd}=0.6$

FIG. 5

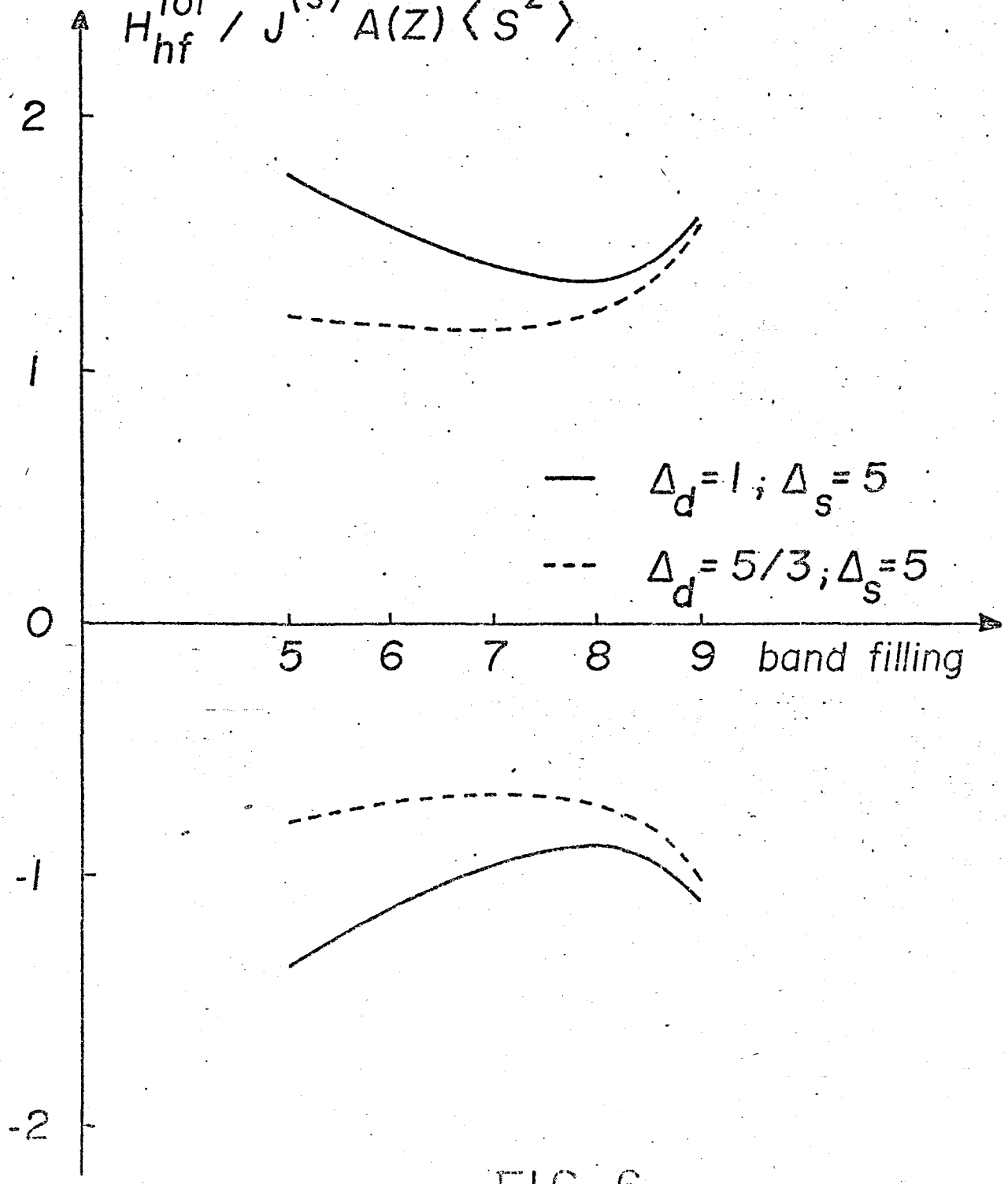
$H_{hf}^{tot} / J^{(s)} A(Z) \langle S^z \rangle$
2
1
0
-1
-2
5
6
7
8
9
band filling
$\Delta_d = 1 ; \Delta_s = 5$
$\Delta_d = 5/3 ; \Delta_s = 5$

FIG. 6

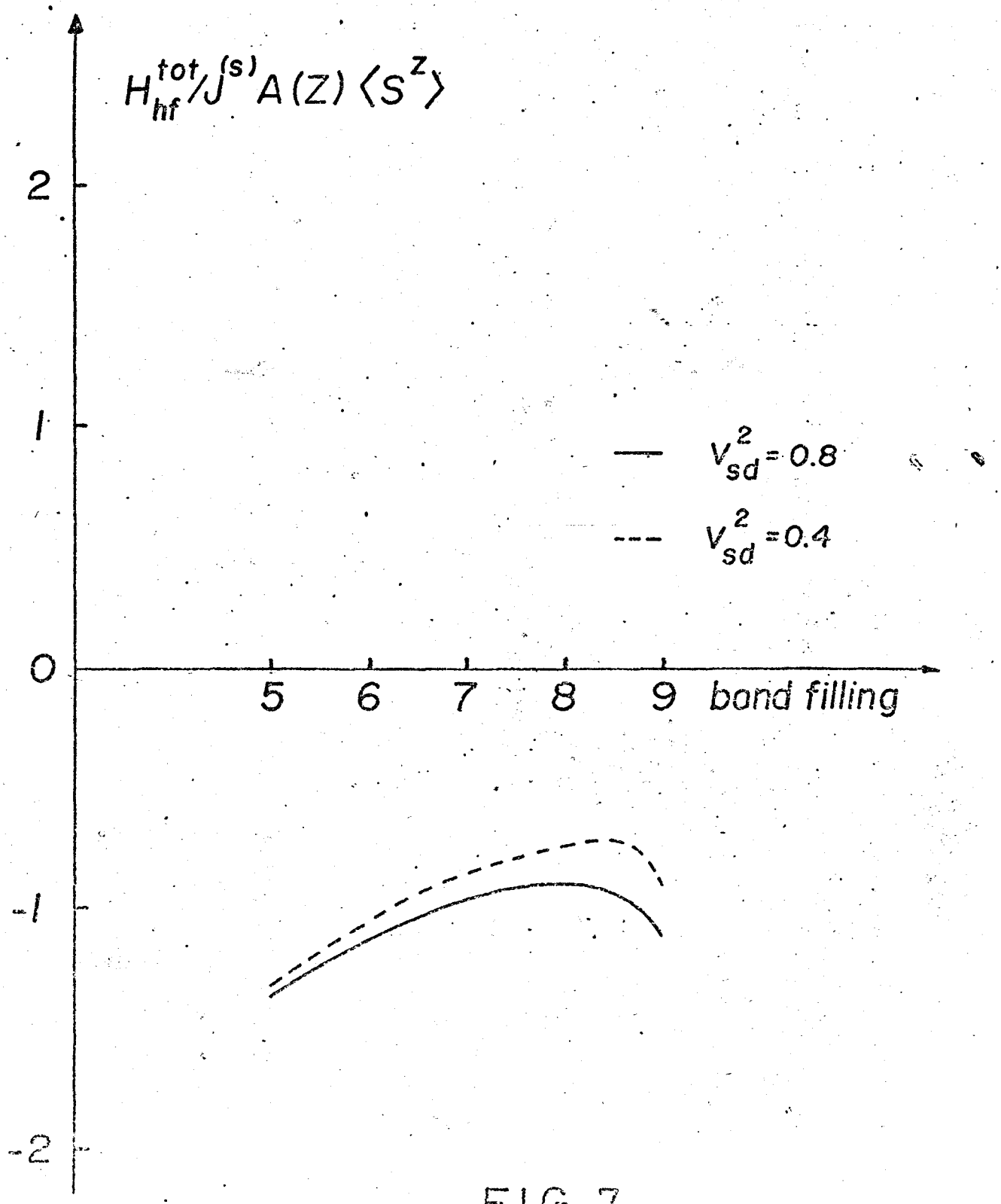
$H_{hf}^{tot}/J^{(s)}A(Z)\langle S^z\rangle$
2
1
0
-1
-2
5
6
7
8
9
band filling
$V_{sd}^2=0.8$
$V_{sd}^2=0.4$

FIG. 7

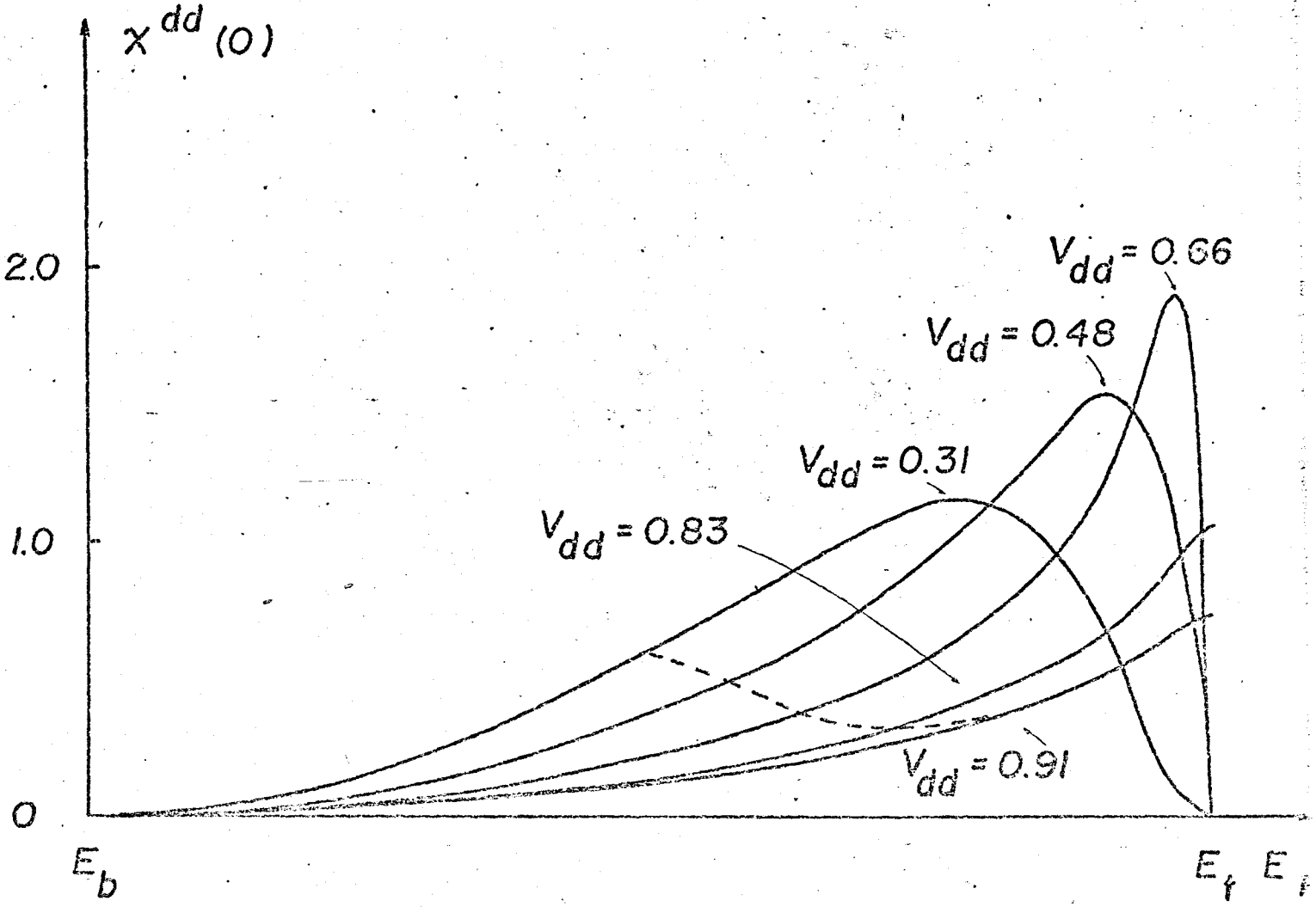


FIG. 8

-1.0
-0.5
0
0.5
1
$H_{hf}^{(s)} / J^{(s)} A(Z) \langle S_z \rangle$
5
6
7
8
9
6
band filling
$J^{(d)} < 0$
$J^{(p)} < 0$

FIG. 9

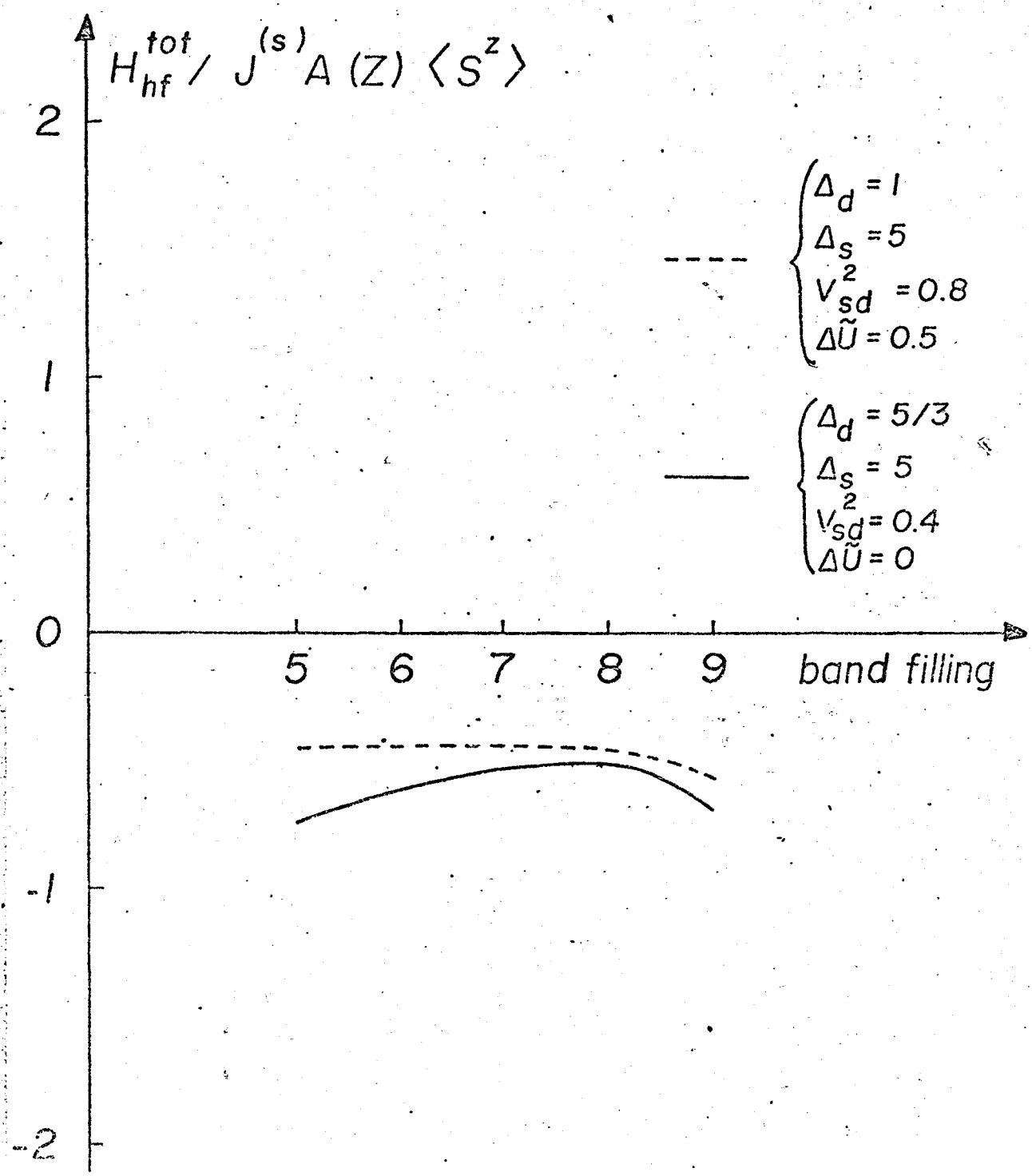
$H_{hf}^{tot} / J^{(s)} A(Z) \langle S^z \rangle$
2
1
0
-1
-2
5
6
7
8
9
band filling
$\Delta_d = 1$
$\Delta_s = 5$
$V_{sd}^2 = 0.8$
$\Delta\tilde{U} = 0.5$
$\Delta_d = 5/3$
$\Delta_s = 5$
$V_{sd}^2 = 0.4$
$\Delta\tilde{U} = 0$

FIG. 10

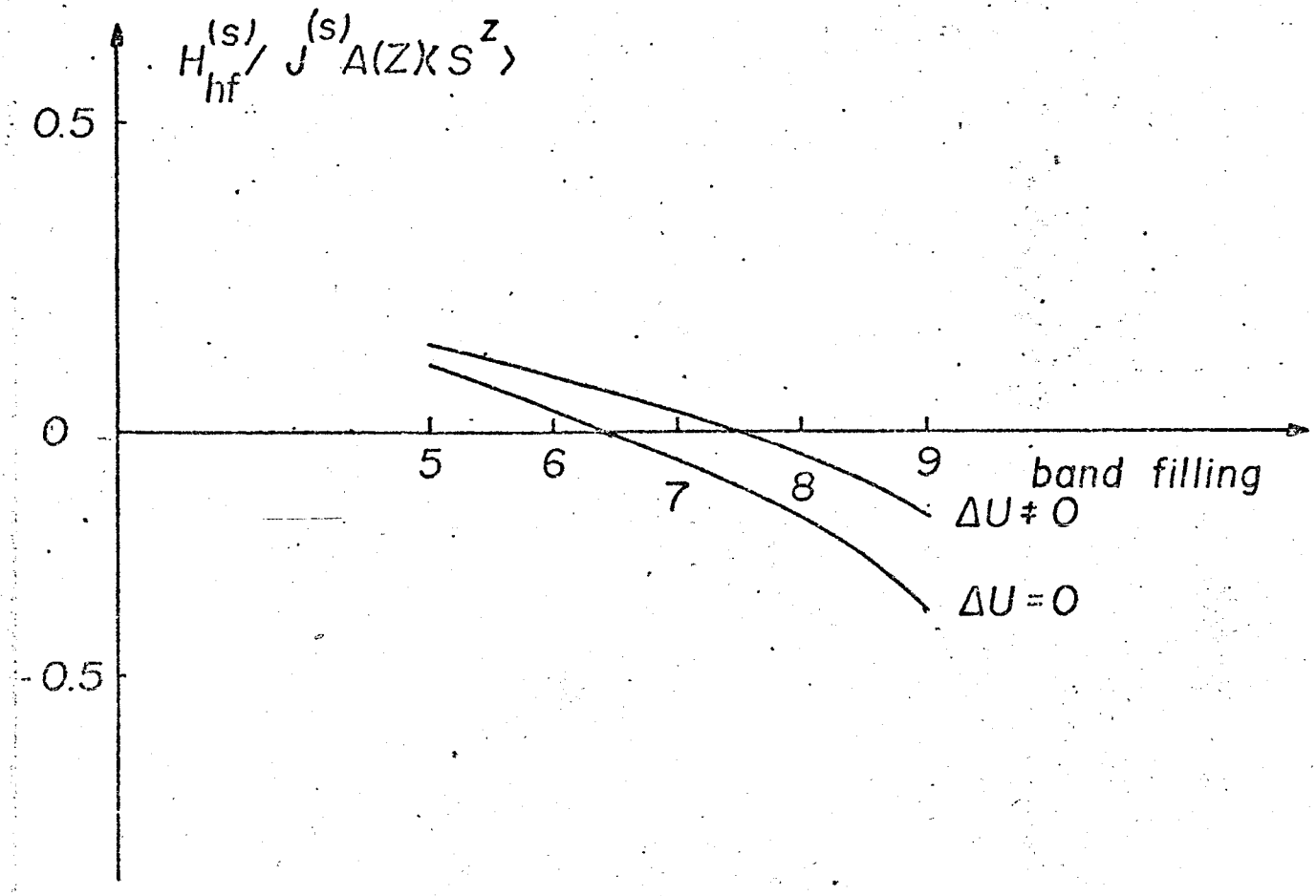
$H_{hf}^{(s)} / J^{(s)} A(Z) \langle S^z \rangle$
0.5
0
-0.5
5
6
7
8
9
band filling
$\Delta U \neq 0$
$\Delta U = 0$

FIG. 11

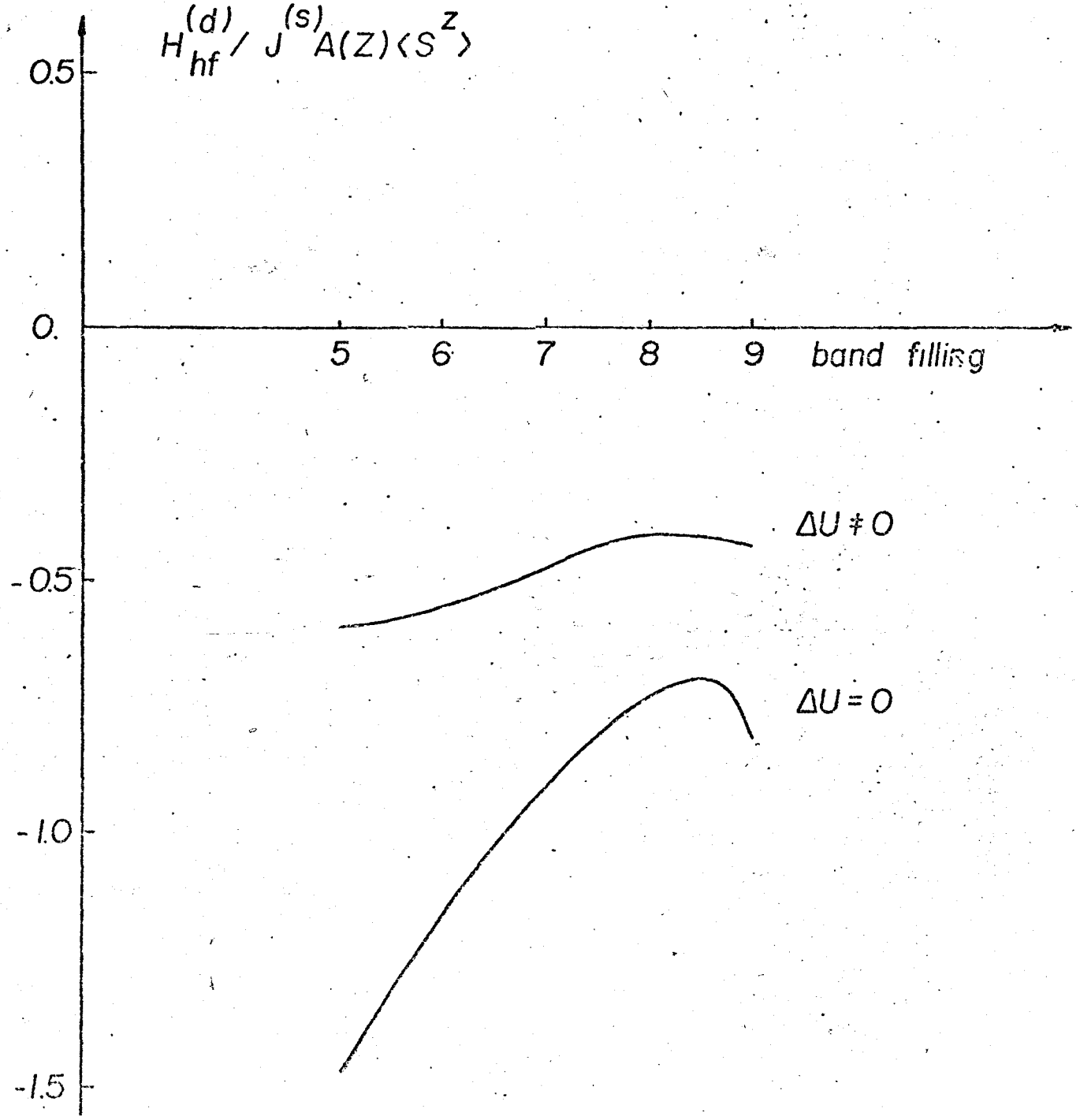
$H_{hf}^{(d)} / J^{(s)} A(Z) \langle S^z \rangle$
0.5
0.
-0.5
-1.0
-1.5
5
6
7
8
9
band filling
ΔU ≠ 0
ΔU = 0

FIG. 12

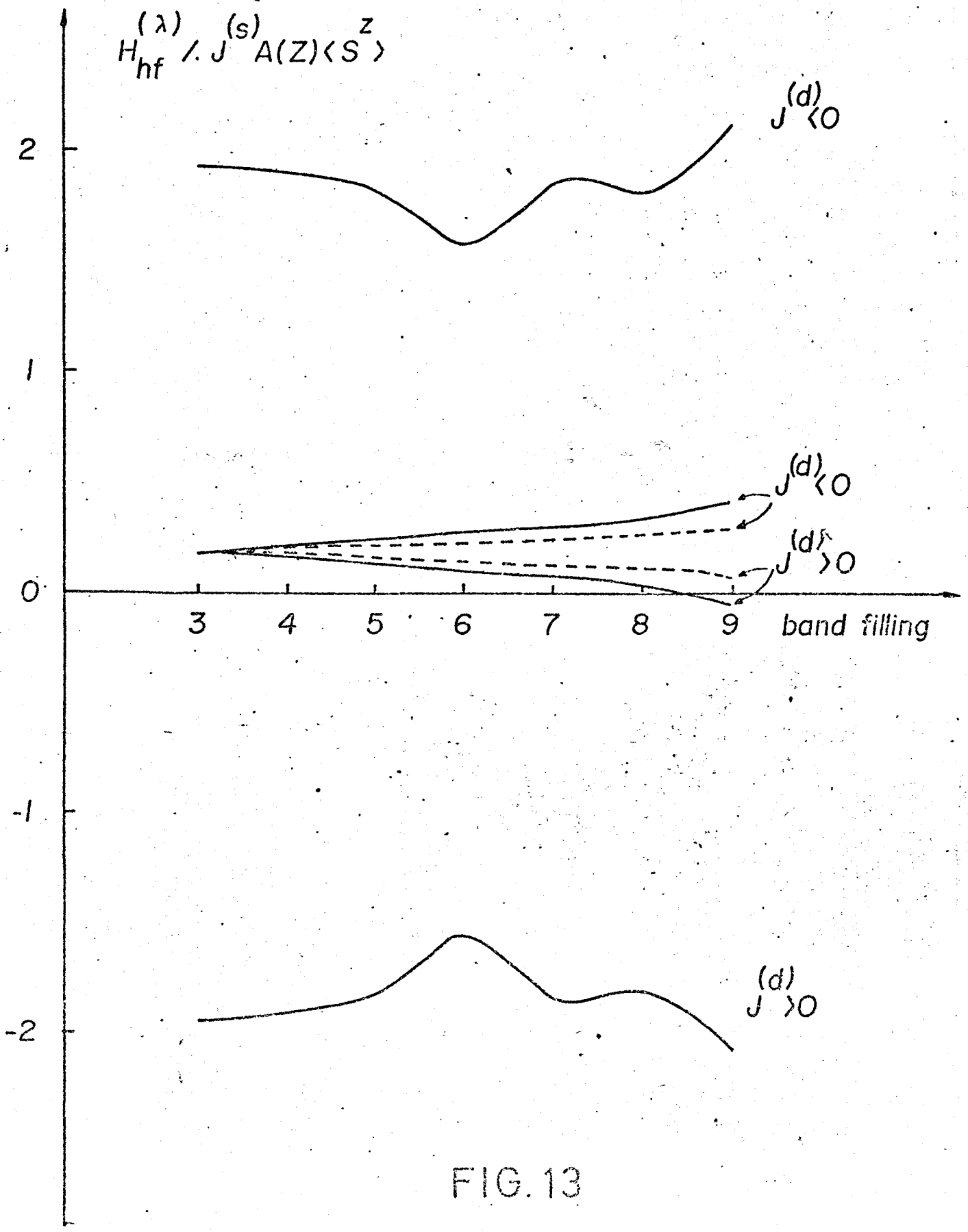
$H_{hf}^{(\lambda)} / J^{(s)} A(Z) \langle S^z \rangle$
2
1
0
-1
-2
3
4
5
6
7
8
9
band filling
$J^{(d)} < 0$
$J^{(d)} < 0$
$J^{(d)} > 0$
$J^{(d)} > 0$

FIG. 13