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HYPERFINE FIELDS OF RARE EARTH IMPURITIES IN TRANSITION HOSTS*

by

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ABSTRACT

We have studied theoretically the hyperfine field at the nucleus of a rare earth impurity dissolved in a transition metal host.

This system is a limiting case of a problem studied by a number of authors (Blandin and Campbell, 1973; Campbell and Blandin, 1975), namely that of the hyperfine field at a non-magnetic impurity spin at a distance $\underset{\sim}{R}_0$ (Heusler alloys). In the case we study, both the polarizing spin and the impurity potential are superposed at the same site. This problem is particularly interesting in the study of the order parameter of the spin glass phase (Young and Stinchcombe, 1976) when the concentration of rare earth impurities is in the corresponding range.

Given the fact that in the Heusler alloys the sign of the hyperfine field may change sign with the non magnetic impurity potential strength, it is necessary to investigate what the sign of the hyperfine field should be in our case.

We have performed numerical computations for a number of model band structure, taking into account the two-band nature of the transition metals and treating the exchange coupling of the impurity spin with the s- and d- electron gas to first order in perturbation. We find that the s- contribution to the hyperfine field may indeed change sign with the impurity potential difference between the rare earth impurity and the matrix. However, the d- contribution does not, and as it is larger, the total hyperfine field remains negative throughout the transition metal series, if the exchange coupling between the d-electron gas and local f-spin is positive.

I. INTRODUCTION

The model due to Blandin and Campbell (Blandin and Campbell, 1973; Campbell and Blandin, 1975) to interpret the hyperfine field at the s-p site Y in the Heusler alloys X_LMnY, consists basically in discussing the effects of a localized charge potential acting on a free electron-like band which is polarized via a local moment placed at a distance $\underset{\sim}{R}_o$ from the strong impurity charge potential.

We have generalized the Blandin-Campbell problem in order to account for a situation where: (i) one must consider a more complicated band structure, namely an s- and d- character conduction band; (ii) the charge and spin perturbations are superposed at the same site.

Experimentally, this situation may be realized in practice when a rare earth impurity (trivalent in general) is diluted in a transition metal host.

A number of spin glass systems, for a suitable range of rare earth impurity concentrations belong to this class of alloys. The measurement of the hyperfine field at the nucleus of the rare earth impurity is a direct way of gaining information on the order parameter of the spin glass phase its magnitude and its temperature dependence. In view of the current interest in the spin glass phase, it is important to have a detailed theory of the self-polarization hyperfine field at the rare earth impurity nucleus in terms of s-(contact) and d-(core) contributions.

In particular, because of the observed change of sign of the hyperfine field at non magnetic impurity sites in Heusler alloys it was both interesting and necessary to investigate the behaviour of the sign of the hyperfine field at the rare earth nucleus in transition metal hosts.

II. THE MODEL

We adopt the following Hamiltonian for a magnetic rare earth impurity embedded in a transition metal-like host:

$$H = H_o + H_{ch}^{imp} + H_{exch}^{imp} + H_{coul.}^{imp} \qquad (1)$$

In (1) H_o describes the non-hybridized s-d bands; H_{ch}^{imp} is the impurity charge potential with s-d and d-d matrix elements; H_{exch}^{imp} corresponds to the exchange coupling of the d- and s- conduction electrons to the local f- moment and H_{coul}^{imp} describes the change ΔU in the Coulomb correlation introduced by the impurity. The reader is referred to Bisch et al. 1976 for notations and definitions of the terms.

We have calculated the total self-polarization hyperfine field in terms of s-(contact) and d-(core) contributions. These contributions are obtained as a function of:

(i) local magnetic responses $\chi^{\alpha\beta}(0)$, $(\alpha,\beta = s,d)$;
(ii) strenght of the usual $J^{(\alpha)}$ $(\alpha = s,d)$ exchange couplings between conduction electrons and the localized f state;
(iii) the hyperfine contact and core parameters $A(Z)$ and A_{cp} (Campbell 1969).

We systematically study as a function of the position of the Fermi level, the influence on the susceptibilities $\chi^{\alpha\beta}(0)$ of the band shapes, the strenght of various d-d scattering matrix elements (with and without d-bound state present), and the influence of local impurity induced s-d mixing potential.

Self-consistent calculations, in order to account for the band filling of the host and the excess charge introduced by the rare earth impurity are also performed.

III. RESULTS

It turns out from our self-consistent calculation, that the s-part of the hyperfine field may change sign as a function of band filling similarly to the s-p or Heusler alloys case (Blandin and Campbell 1973; Campbell and Blandin 1975).

However, as expected, the d-part contributes a large magnetic susceptibility $\chi^{dd}(0)$ and therefore the core polarization dominates, the total hyperfine field being negative.

The influence of the parameters of the model has been studied in detail and situations that could be differentiated experimentally are suggested (see figures 1 and 2). Figures 1 and 2 summarize some of the results.

IV. CONCLUSION

As a final comment it has been proposed by Rettori et al. 1973 in order to understand bottlenecked systems (EPR experiments), that the $J^{(d)}$ coupling may be negative (usual

Heisenberg coupling to next neighbours). If this is true, our results may suggest a positive self-polarization hyperfine field which could be a good experimental check of the negative $J^{(d)}$ coupling assumption.

Acknowledgements

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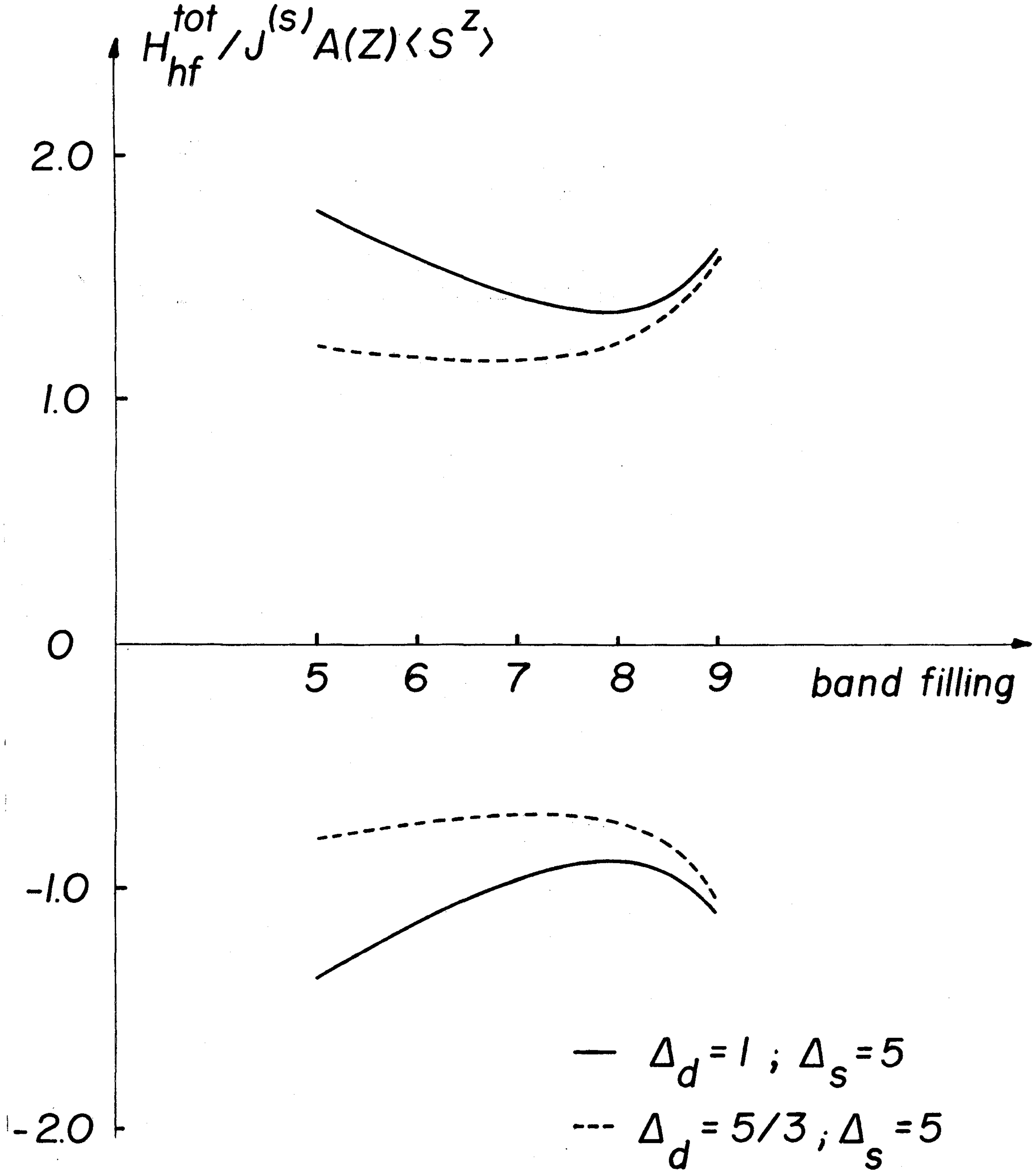
FIGURE CAPTIONS

Figure 1. Qualitative description of period effect e.g. rare earth impurities in 4d and 5d metals.
One shows the total self polarization field for two different d-band widths, the s-band width being kept constant. Two situations are shown: for $J^{(d)} > 0$ and $J^{(s)} > 0$ one has negative hyperfine field whereas for $J^{(d)} < 0$, $J^{(s)} > 0$ (Rettori et al. 1973) one has positive total hyperfine field. One sees that the minimum (maximum) value shifts from the middle of the series to the end of the series when one increases the d-band width. The significant difference in hyperfine fields in 4d and 5d hosts turns out to be expected around the middle of the series, when the local change in Coulomb correlation ΔU is disregarded.

Figure 2. s-(contact) and d-(core) contributions to the hyperfine field as a function of the local correlation $\Delta U (=0$ and $\neq 0)$.

Figure 2(a). show the main features of the s-like contribution for the self polarization field, for the case of $J^{(d)} > 0$, $J^{(s)} > 0$. One sees the possibility of a change in sign which shows a close resemblance to the usual results discussed by several authors (Campbell and Blandin 1975; Campbell 1969).

Figure 2(b). shows the d-contribution for the hyperfine field, $(J^{d} > 0,\ J^{s} > 0)$, which is dominant, thus determining the sign of the total field.



$H_{hf}^{tot}/J^{(s)}A(Z)\langle S^z\rangle$
2.0
1.0
0
-1.0
-2.0
5
6
7
8
9
band filling
— $\Delta_d = 1$; $\Delta_s = 5$
--- $\Delta_d = 5/3$; $\Delta_s = 5$

FIG. 1

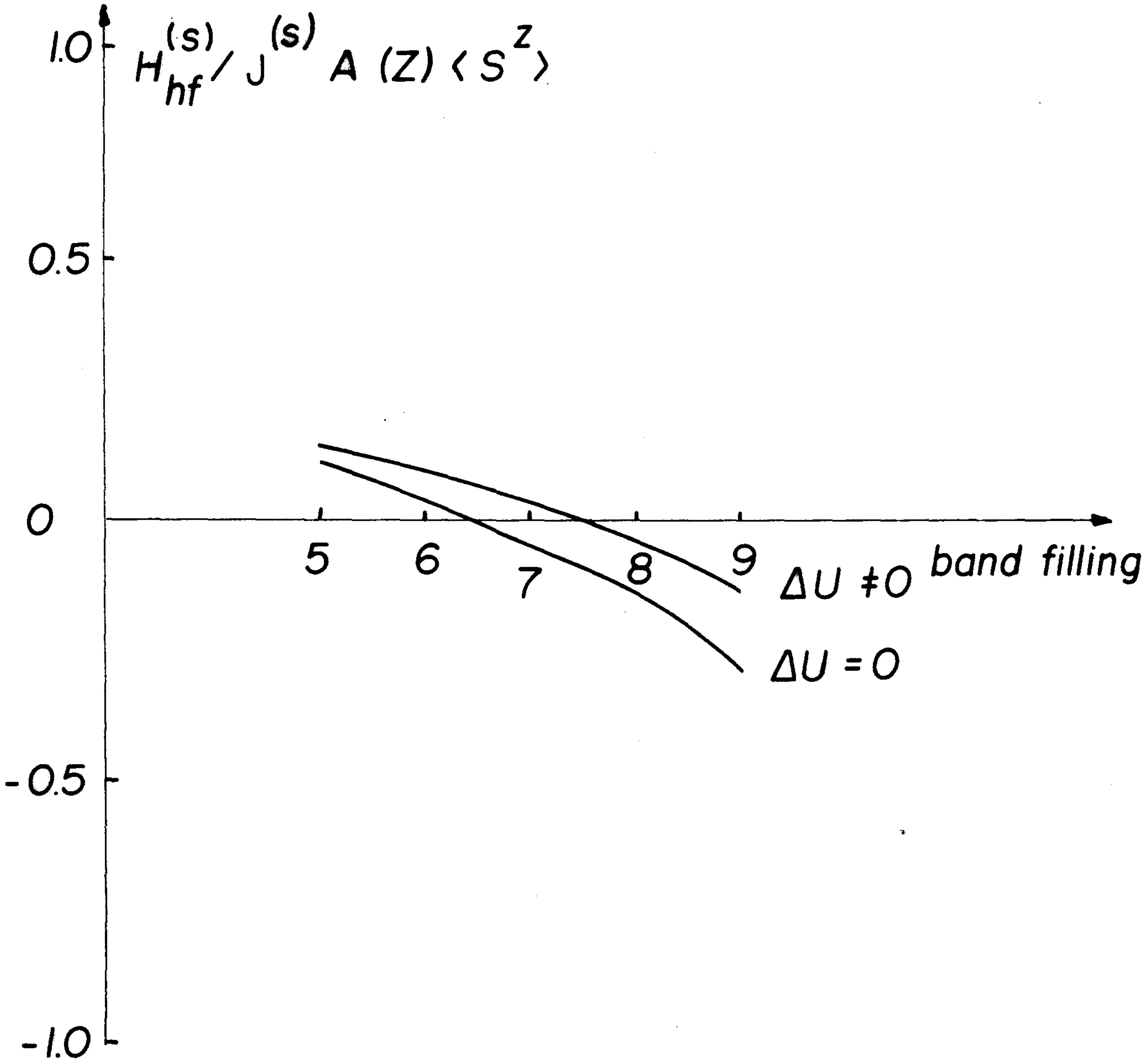
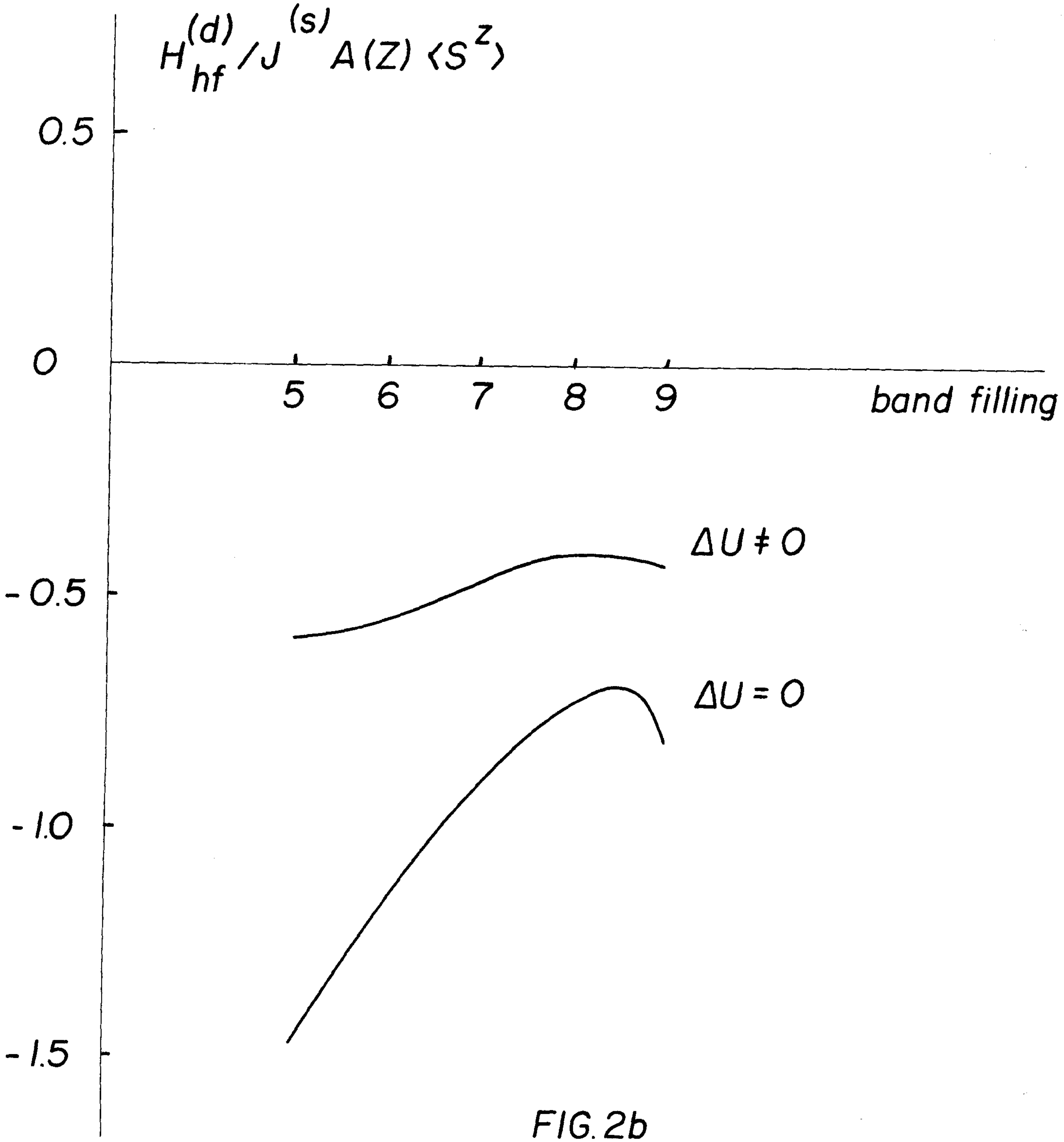

$H_{hf}^{(s)}/J^{(s)}A(Z)\langle S^z\rangle$
1.0
0.5
0
-0.5
-1.0
5
6
7
8
9
band filling
ΔU ≠ 0
ΔU = 0

FIG. 2a



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

FIG. 2b