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## CALCULATION OF THE SPIN WAVE ENERGY OF IRON, COBALT AND NICKEL

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**Résumé.** — On a calculé les énergies d'ondes de spin dans le fer, le cobalt et le nickel dans la limite des grandes longueurs d'onde et dans l'approximation de la phase aléatoire, en utilisant les résultats des calculs de structure de bande. On donne l'expression de l'énergie et le critère de stabilité de l'état fondamental ferromagnétique à l'aide de la fonction  $M(\epsilon)$ , qui est une intégrale de surface dépendant du gradient de l'énergie d'une particule isolée. Les résultats obtenus montrent l'importance possible de la bande s-p, qui peut contribuer à la stabilisation de l'état fondamental ferromagnétique.

L'accord entre nos calculs et les valeurs expérimentales est très bon pour le nickel. Pour le cobalt et pour le fer, les valeurs calculées sont beaucoup plus petites que les valeurs observées.

**Abstract.** — The spin wave energies for iron, cobalt and nickel are computed in the long wave length limit and in the random phase approximation, using the results of band structure calculations. The energy expression and the criterion for the stability of the ferromagnetic ground state are given in terms of a function  $M(\epsilon)$ , a surface integral involving the gradient of the single particle energy. The results obtained indicate the possible importance of the s-p band in helping to stabilize the ferromagnetic ground state.

Agreement with experiemntal values of the spin wave energy is very good for nickel, but for cobalt and iron the calculated values are much smaller than those observed.

**I. Introduction.** — Several calculations of the spin wave energy of ferromagnetic iron and nickel using the random phase approximation have been published [1-4]. In the long wavelength limit the spin wave energy takes the form  $Dq^2$  for a given direction of the wave vector  $q$ . For a cubic crystal  $D$  is independent of this direction and in RPA, considering only intraatomic interactions and intraband spin flipping,  $D$  at 0 °K is given by [5], [4]

$$D = \frac{1}{3n} \sum_{\lambda} \left\{ \frac{1}{2} \left( \sum_{\epsilon_{\lambda k} < \epsilon_{\lambda+}} \nabla^2 \epsilon_{\lambda k} + \sum_{\epsilon_{\lambda k} < \epsilon_{\lambda-}} \nabla^2 \epsilon_{\lambda k} \right) - \frac{1}{\Delta_{\lambda}} \left( \sum_{\epsilon_{\lambda k} < \epsilon_{\lambda+}} |\nabla \epsilon_{\lambda k}|^2 - \sum_{\epsilon_{\lambda k} < \epsilon_{\lambda-}} |\nabla \epsilon_{\lambda k}|^2 \right) \right\}. \quad (1)$$

Here  $n = n_+ - n_-$ , the excess number of electrons, and  $\epsilon_{\lambda \pm} = \mu \pm \frac{1}{2} \Delta_{\lambda}$ , where  $\Delta_{\lambda}$  is the single particle exchange splitting in the band  $\lambda$ . For a non-cubic crystal such as HCP cobalt, (1) gives the mean value of  $D$  for any three mutually orthogonal directions. The value of  $D$  along a given axis, say the c-axis in cobalt, may also be calculated.

In the present calculation we adopt a single particle exchange splitting  $\Delta$  common to all bands, determined from the density of states  $N(\epsilon)$  and the observed  $n$ . Callaway and Zhang [6] calculated  $\Delta_{\lambda}$  a priori for nickel using a t-matrix approximation, but this low density approximation is inapplicable to cobalt and iron. With these simplifications and using Green's theorem (1) becomes

$$D = \frac{1}{3n} \left\{ \frac{1}{2} [M(\epsilon_+) + M(\epsilon_-)] - \frac{1}{\Delta} \int_{\epsilon_-}^{\epsilon_+} M(\epsilon) d\epsilon \right\}, \quad (2)$$

where

$$M(\epsilon) = \frac{\Omega}{8\pi^3} \sum_{\lambda} \int_{\epsilon_{\lambda k} = \epsilon} |\nabla \epsilon_{\lambda k}| dS. \quad (3)$$

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This function  $M(\epsilon)$  is analogous to the usual density of states function  $N(\epsilon)$  except that the gradient appears in the numerator and thus it contains no Van Hove singularities. In (2) no second derivatives of  $\epsilon_{\lambda k}$  occur so that  $D$  may be calculated more accurately than in earlier calculations. Clearly from (2),  $D$  is proportional to the algebraic area between the curve  $M(\epsilon)$  and the straight line joining points on the curve at  $\epsilon_+$  and  $\epsilon_-$ , see figure 1. Thus in this case, if  $M(\epsilon)$  lies predominantly below this line,  $D > 0$ , i. e. the ferromagnetic ground state is stable.

To calculate the band structure  $\epsilon_{\lambda k}$  needed in (3) the model Hamiltonian method proposed by Hubbard [7] is used for BCC iron and FCC nickel, and that generalized [8] to several atoms in the unit cell is used for HCP cobalt. The band structure of the 3d-bands of BCC iron without considering the hybridization with the 4s-4p bands is also calculated by using the Slater-Koster LCAO interpolation method [9]. This is done in order to compare the results with those obtained by Thompson et al. [2] and to study the effect of the hybridization. Results are obtained for two different crystal potentials for each metal.

**II. Details of the calculations.** — (a) BCC IRON WITHOUT 4s-4p BANDS. — Energy values at 285 k-points in 1/48th of the Brillouin zone were calculated by using the LCAO interpolation method. In order to obtain  $M(\epsilon)$  and  $N(\epsilon)$ , the linear interpolation scheme developed by Lipton and Jacobs [10] was adopted. The LCAO interpolation parameters were chosen to fit (1) the minority spin band in ref. [11] and (2) a band averaged over the two spins in [11]. Thompson et al. [2] also used a fit to the averaged band, but obtained a negative value of  $D$ .  $M(\epsilon)$  for the parameters (2) is shown in figure 1a. Table I gives effective masses  $m^*$  such that  $D = \hbar^2/2 m^*$ ; for iron without 4s-4p bands,  $D$  is thus almost zero.

(b) BCC IRON WITH 4s-4p BANDS. — Hubbard's

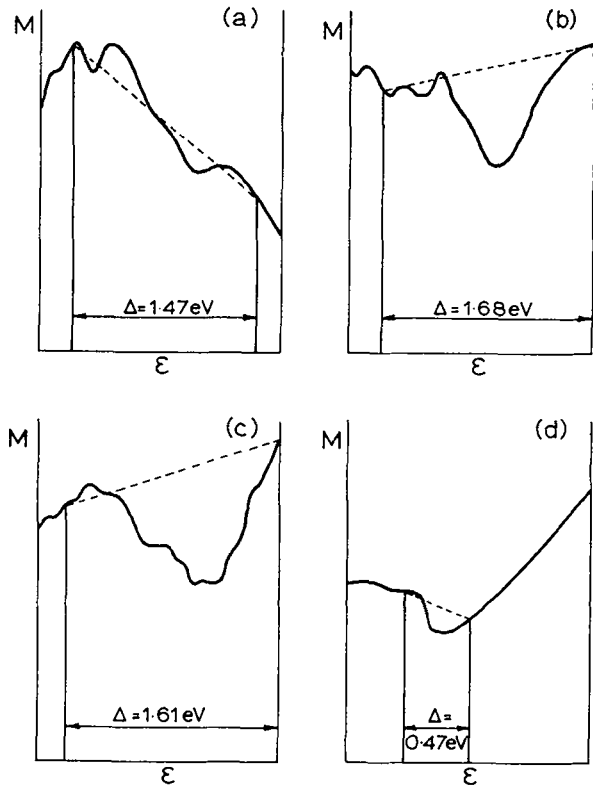


FIG. 1. — The function  $M(\epsilon)$  for (a) Fe without s-p band, (b) Fe with s-p band, (c) Co, (d) Ni. The dotted lines join points on the curves at  $\epsilon_+$  and  $\epsilon_-$ .

method [7] is used with 7 plane waves. In order to compare the results with those obtained in the previous section, the potentials used are (1') that of the minority spin-band in [11], and (2') that averaged between the two spin-bands. The function  $M(\epsilon)$  for the potential (2') is shown in figure 1b, and the  $m^*$  values are shown in table I. There is not much difference between the main features of the density of states curve with and without the 4s-4p bands. Because the numerous Van Hove singularities in  $N(\epsilon)$  are due to d-states at high symmetry points, such points are not greatly affected by 4s-4p states. On the other hand,  $M(\epsilon)$  reflects the derivatives of the energy

curve, so that  $M(\epsilon)$  is changed markedly by introducing the 4s-4p bands. This explains the marked influence of these bands on  $m^*$ , and shows that they help to stabilize the ferromagnetic ground state.

(c) HCP COBALT. — The generalized model Hamiltonian method [8] with 8 plane waves is used in order to calculate energy values at 225 k-points in 1/24th of the Brillouin zone. In order to obtain a more reasonable relation between the 4s-4p bands and the 3d-bands than in the original calculations [12], the 4s-4p bands were shifted by amounts (1) 0.54 eV and (2) 1.1 eV to the lower energy side. The function  $M(\epsilon)$  for (1) is shown in figure 1c and  $m^*$  values are shown in table I. When the upper s-like bands are neglected,  $D$  is reduced to  $\frac{1}{4}$  of the original value. The d-component of the s-like bands at  $\epsilon_+$  is about  $\frac{2}{3}$ , so that these bands should not be omitted in the calculation of  $D$ . Table I contains the average  $D$  given by (1) as well as the calculated value along the c-axis relevant to the measurements [14]. The calculated anisotropy in  $D$  is thus small.

(d) FCC NICKEL. — Hubbard's method [7] with 4 plane waves is used to calculate energy values at 505 points in 1/48th of the Brillouin zone. The potentials used are (1) that of the minority spin band, and (2) that of the paramagnetic band in [13]. The function  $M(\epsilon)$  for potential (1) is shown in figure 1d and  $m^*$  in table I. For nickel  $M(\epsilon)$  due to the s-like band happens to be linear and there is no contribution from that band to  $D$ .

III. Discussion. — The results of the calculations are given in table I together with those of previous calculations [1-4], and experimental values [14]. The agreement between experiment and the calculated value is very good for nickel, but for iron and cobalt the calculated spin wave energies are much smaller than those observed. This result may be due to the inapplicability of RPA in the form leading to (1). A model suitable for iron and cobalt should include explicit consideration of Hund's rule interactions.

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TABLE I

	Fe (1)	Fe (2)	Fe (1')	Fe (2')	Co (1)	Co (2)	Ni (1)	Ni (2)
$m^*/m$ (calc.)	- 286	+ 1 000	62.5	47.6	{ 26.1 23.8 (3)	{ 21.4 19.8 (3)	14.7	13.3
$m^*/m$ (exp.)		13.1				7.5 (3)		10.2
$m^*/m$ (previous)		negative				35 (3)	34	30 $\pm$ 10
Ref.		[2]				[3]	[1]	[4]

Explanation (refer to text): Fe (1), (2) d-band only with different LCAO parameters; (1'), (2') with s-p band with different potentials. Co (1) bands shifted by 1.1 eV; (2) bands shifted by 0.54 eV; (3) along c-axis. Ni (1), (2) different potentials.

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