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## MULTI-ORBITAL CPA CALCULATION OF SPIN WAVE ENERGIES IN NICKEL ALLOYS

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**Abstract.** - Calculations of the spin wave stiffness constant in ferromagnetic  $\text{Ni}_{1-x}\text{Co}_x$  and  $\text{Ni}_{1-x}\text{Fe}_x$ , with  $0 < x < 0.5$ , are based on a coherent potential approach to a tight-binding d-band model with both diagonal and off diagonal disorder. The results differ significantly from those of earlier work using the virtual crystal approximation and the agreement with experiment is good for NiCo but poor for concentrated NiFe alloys.

### 1. Introduction

Existing theoretical work [1-6] on the spin-wave stiffness constant  $D$  in alloys is based on either unrealistic one-band models or the multi-band Wannier scheme with the assumption that electrons interact only when they occupy Wannier functions centred on the same site. A more realistic interaction is one which is onsite in a basis of atomic orbitals rather than Wannier functions. Using this model Edwards and Muniz have used the random phase approximation to derive a formula for  $D$  which they have applied to Ni and Fe and, using the virtual crystal (VC) approximation, to their alloys [7]. In the present work we calculate  $D$  for transition metal alloys taking into account the orbital degeneracy and treating the disorder within the more adequate coherent potential approximation.

### 2. Theory

The alloy Hamiltonian we use is a multi-orbital tight-binding model given by

$$H = \sum_{i\mu\sigma} \varepsilon_i c_{i\mu\sigma}^\dagger c_{i\mu\sigma} + \sum_{ij} \sum_{\mu\nu\sigma} t_{ij}^{\mu\nu} c_{i\mu\sigma}^\dagger c_{j\nu\sigma} + H_{\text{int}} \quad (1)$$

where  $c_{i\mu\sigma}^\dagger$  creates an electron in an atomic state labelled by the site  $\mathbf{R}_i$ , orbital  $\mu$  and spin  $\sigma$  and  $H_{\text{int}}$  contains only spin invariant intra-atomic interactions. We assume that the hopping integrals satisfy  $t_{ij}^{\mu\nu} = \alpha_i \tilde{t}_{ij}^{\mu\nu} \alpha_j$ , where  $\tilde{t}_{ij}^{\mu\nu}$  is independent of the atomic species on sites  $i$  and  $j$ .  $\varepsilon_i$  are the site energies. Following Edwards and Hill [4] we approximate the exact formula for  $D$  [8] by applying the Hartree-Fock (HF) approximation to the spin current response function which appears in it and by using the coherent potential (CP) approximation. Thus for a random alloy with an underlying cubic lattice we find

$$D = \frac{1}{6\pi(N_\uparrow - N_\downarrow)} \left\{ \sum_{\mathbf{k}} \sum_{\mu\nu} B_{\mu\nu}(\mathbf{k}) \times \int dE f(E) \sum_{\sigma} \text{Im} G_{\mu\nu}^{\sigma}(\mathbf{k}, E) + 2 \sum_{\mathbf{k}} \sum_{\mu\nu} \sum_{\mu'\nu'} A_{\mu\nu}(\mathbf{k}) \cdot A_{\mu'\nu'}^*(\mathbf{k}) \times \int dE f(E) \text{Im} [G_{\nu\mu'}^{\uparrow}(\mathbf{k}, E) G_{\nu'\mu}^{\downarrow}(\mathbf{k}, E)] \right\} \quad (2)$$

where  $f(E)$  is the Fermi function,  $B_{\mu\nu}(\mathbf{k})$  and  $A_{\mu\nu}(\mathbf{k})$  are, respectively, the Laplacian and the gradient of the lattice Fourier transform  $V_{\mu\nu}(\mathbf{k})$  of the  $\tilde{t}_{ij}^{\mu\nu}$ , and  $G_{\mu\nu}^{\sigma}(\mathbf{k}, E)$  is the time-Fourier transform of a one-electron Green function, defined as the HF-CP approximation to the configuration average of

$$G_{\mu\nu}^{\sigma}(\mathbf{k}, t) = -\frac{i}{\hbar} \theta(t) \langle [\tilde{c}_{\mathbf{k}\mu\sigma}(t), \tilde{c}_{\mathbf{k}\nu\sigma}^\dagger]_+ \rangle. \quad (3)$$

Here  $\tilde{c}_{\mathbf{k}\mu\sigma} = \sum_i \alpha_i \exp[-i\mathbf{k} \cdot \mathbf{R}_i] c_{i\mu\sigma}$ .

In obtaining (2) we approximate the configuration average  $\langle G^\dagger G^\dagger \rangle_c$  by  $\langle G^\dagger \rangle_c \langle G^\dagger \rangle_c$ . This approximation is expected to be valid for alloys such as Ni-Co and Ni-Fe, in which the effect of disorder on the majority spin states is not pronounced so that  $D^\uparrow$  is approximately independent of configuration. For a pure metal (2) reduces to the result of Edwards and Muniz [7].

### 3. Application to Ni-Co and Ni-Fe alloys

Using expression (2) we calculate  $D$  for FCC  $\text{Ni}_{1-x}\text{Co}_x$  and  $\text{Ni}_{1-x}\text{Fe}_x$  alloys for  $x < 0.5$ . We consider d-orbitals only and parametrize  $H_{\text{int}}$  assuming that  $\langle i\mu\sigma, i\nu\sigma' | v | i\gamma\sigma', i\eta\sigma \rangle = U_i \delta_{\mu\eta} \delta_{\nu\gamma}$ , where  $v$  is an effective electron-electron interaction. We keep nearest-neighbour hopping only and take  $\tilde{t}$  from Zornberg's PSI parametrization [9] with  $\alpha_{\text{Ni}} = 1$ .

The origin of the energies is set at  $\varepsilon_{\text{Ni}}$ . We choose  $U_{\text{Ni}} = 0.062 \text{ Ry}$ , which gives for pure Ni the value  $D_{\text{Ni}} = 525 \text{ meV \AA}^2$  measured by Hennion *et al.* [5]. To obtain the true value of  $D_{\text{Ni}}$ , corresponding to the observed small- $q$  limit [10] we should really use  $U_{\text{Ni}} = 0.052 \text{ Ry}$  [7]. However, since we wish to compare with the triple axis neutron data of Hennion and Hennion [11, 12] for alloys, it may be argued that  $U_{\text{Ni}} = 0.062 \text{ Ry}$  is more appropriate. The values of  $\alpha_{\text{Co}}$  and  $\alpha_{\text{Fe}}$  are estimated as 1.1 and 1.2, respectively. The remaining parameters, namely  $\varepsilon_{\text{M}}$  and  $U_{\text{M}}$  ( $\text{M} = \text{Co, Fe}$ ), are determined so as to fit the observed local magnetic moments  $\mu_{\text{Ni}}$  and  $\mu_{\text{M}}$  as a function of the alloy composition. The values we obtain are  $\varepsilon_{\text{Co}} = 0.017 \text{ Ry}$ ,  $U_{\text{Co}} = 0.067 \text{ Ry}$ ,  $\varepsilon_{\text{Fe}} = 0.094 \text{ Ry}$ , and  $U_{\text{Fe}} = 0.059 \text{ Ry}$ . The number  $n_{\text{d}}$  of d-electrons per atom we use are 9.44, 8.40, and 7.20 for Ni, Co, and Fe, respectively. In solving the CP equations we decouple the  $e_{\text{g}}$  and  $t_{2\text{g}}$  equations according to Kirkpatrick

*et al.* [13]. The  $k$ -space integrations are performed using the linear analytic tetrahedron method with 1536 tetrahedra in the irreducible part of the Brillouin zone. Results for  $D$  as a function of  $n_{\text{d}}$  are presented in figures 1a and 1b for Ni-Co and Ni-Fe alloys, respectively. The results are compared with experiment and with the multi-orbital VC result of Edwards and Muniz [7]. In the case of Ni-Co the agreement between the present result and the experiment is remarkable. The results for Ni-Fe alloys are sensitive to  $\alpha_{\text{Fe}}$ , but for reasonable choices of this parameter the calculated values of  $D$  for  $x > 0.05$  always lie far below the existing measured values. Possibly sp bands must be included as is known to be essential for pure BCC Fe [7]. However it would be interesting to extend the small  $q$  measurement of reference [10] to alloys.

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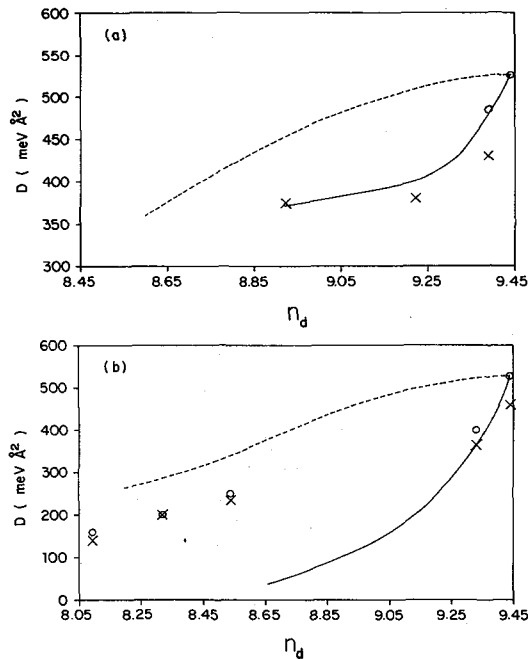


Fig. 1. — Spin wave stiffness constant  $D$  for Ni-Co (a) and Ni-Fe (b) alloys as a function of the number  $n_{\text{d}}$  of d-electrons per atom. Full curve: present result; dashed curve: VC result [4]. Experimental data are represented by (o) ( $T = 4.2 \text{ K}$ ) and (x) (room temperature) [12, 13].

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