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FERROMAGNETIC EXCITATIONS IN HEXAGONAL COBALT (*)

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Abstract. — The results of a multiple band calculation of the magnon energy and Stoner excitations for hcp cobalt, based upon a tight-binding representation of the d-band structure, are presented and the role of a wave vector dependent electron interaction in determining the exchange stiffness of cobalt is discussed. An upper limit on the intra-atomic contribution to the exchange stiffness is found to lie significantly below the experimental value and accordingly it is found necessary to include interatomic exchange to obtain agreement with experiment. The magnon dispersion relation and Stoner excitations in the principal axis directions are presented for a band splitting of .91 eV and interatomic (intercellular) exchange of 16 meV.

Spin wave resonance and inelastic neutron scattering experiments have provided valuable experimental information on the excited spin states of the ferromagnetic 3d transition metals. With the increase in understanding of the electronic structure of these materials, it has become possible to attempt theoretical calculations of the low energy portions of these states. Various forms of the itinerant electron model have been taken as the basis of studies of fcc nickel [1-4] and bcc iron [5]. We report here some interesting results obtained in an extension of this work to include cobalt.

The band structure of hcp cobalt [6-9] is inherently more complicated than that of iron or nickel due to its two atoms per unit cell. Since each atom gives rise to five 3d states the band structure for Co contains ten 3d bands. For a calculation of the magnon energy (and Stoner excitations) it is necessary either to determine these bands from first principles or to obtain a good facsimile by fitting to an existing calculation. In our treatment we fitted the APW energy bands of Hodges and Ehrenreich [7] using the Slater-Koster interpolation scheme with nearest-neighbor interactions [10, 11]. Emphasis was placed on getting a good fit at the higher energy states and as is implied band hybridization was neglected. We assumed that the majority spin 3d bands (10) were entirely filled (5 electrons per atom) while the minority spin bands (10) contained 1.56 holes per atom. It was determined that five hole bands were involved. The energy bands were then split by an amount $\Delta$ such that the configuration for the ferromagnetic species was as is shown in Figure 1. $\Delta$ was treated as an arbitrary parameter limited only by the condition that the ferromagnet be strong.

Our original calculations of the magnon energy $\hbar\omega(q)$ were made using the random phase approxima-


FIG. 1. — Tight-Binding Density of States for Ferromagnetic hcp Cobalt. The majority spin electrons fill all states in majority 3d bands while minority spins allow for 1.56 holes per atom. Five hole bands are involved in determining the calculated magnetic properties. The exchange splitting $\Delta$ is treated as a parameter.
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...isotropic for small wave vectors. From these results it appears unlikely that the acoustical branch along the [001] direction will ever intersect the continuum. We expect, however, intersections in the basal plane along the [110] and [100] directions at about $q_0/\pi = 1$. The exact position of the intersection is dependent upon the value of the band splitting. In a more general treatment we expect to find optical modes in addition to the acoustical mode presented here. These higher energy modes are absent in our treatment due to our assumption of band independent interactions which effectively converts our problem into that for a single band.

References