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EFFECT OF MAGNETIC DISORDER ON THE SPECTRAL DENSITY OF THE d BAND IN FERROMAGNETIC METALS

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Abstract. — It is shown that previous calculations of the spectral density of an extra hole or electron in Fe and Ni can be parametrized with a simple CPA in terms of an exchange splitting parameter and level position in the band both measured in the unit of an effective band width even in the presence of the short range order.

The spin-polarized angle-resolved photoemission experiments [1-3] on nickel and iron which measure the spectral density of a hole of given wave vector and spin in the valence bands convoluted with an apparatus resolution function have revealed, for example that the spectral density at $\Gamma'_{25}$ of the minority spin in iron tends to have a double peak structure near $T_c$ with a secondary peak at the position of the peak of the corresponding spectral density of the majority spin, which is situated at a lower energy. In the case of nickel, on the other hand, the peaks for both spins seem to merge into a single peak at $T_c$ shifting with temperature while keeping a single peak structure.

Meanwhile, calculations with the disordered-local-moment model simulating iron [4-6] have shown that the temperature dependence of the spectral density varies strongly with the choice of wave vector and spin; for example, those at $H_{25}$ and $H_{12}$ will merge into a single peak above $T_c$, while those at $\Gamma_{12}$ remain double peaked even above $T_c$. In the case of $\Gamma'_{25}$ mentioned above the correlation among near neighboring magnetic moments is predicted to affect the spectral density to the extent that one can deduce a quantitative estimate of the correlation by fitting the calculation to the experimental data [5]. Hasegawa [7] has carried out a calculation based on the functional integral theory for nickel and iron to obtain results consistent with the experiment on nickel and similar to those of previous disordered-local-moment model calculations for iron. No detailed discussions, however, have been given so far on the mechanism underlying the variety of the behaviour of the spectral density.

The previous calculations take into account the effect of magnetic disorder by use of the coherent potential approximation [4, 6, 7] or a method capable of taking into account the correlation among near neighbouring moments [5]; this proved to be equivalent to CPA in the absence of it [5]. In order to show that the variety of the temperature variation of the spectral density arises from a quite general origin, independent of details of the electronic structure, we carry out a calculation of the spectral density with a single band tight binding model with assumptions equivalent to the disordered-local-moment model; the potential of each atom is assumed to be spin dependent as given by $\pm \psi_{\alpha\gamma}$ with $\psi_{\alpha\gamma} > 0$, where $+$ and $-$ signs apply to electrons of minority and majority spin, respectively, for atoms having their magnetic moment parallel to bulk magnetization; the sign is reversed if the magnetic moment is antiparallel. We assume further a Lorentzian or bell shape function to represent the state density in the absence of magnetic disorder. We can reproduce then quite accurately the results of previous calculations which take account of details of the electronic structure, concluding that we can parametrize the spectral density for a given average magnetization by three parameters, the exchange splitting $w_{\text{ex}}$, the effective width of the band (for example, the half-width of the Lorentzian state density) and the energy position of the level in the band.

For example, the spectral density of the level near the center of the band tends to have a double peak structure even at $T_c$ if the exchange splitting is sufficiently large compared to the effective width. On the other hand, the minority spin level in a lower half of the band, or the majority spin level in the upper half, tends to join its counterpart of opposite spin with increasing temperature, shifting towards it as a single peak if the level position is sufficiently remote from the center and the exchange splitting is relatively small, while the temperature variation of the counterpart is relatively small. The development of a secondary peak at the position of opposite spin near $T_c$ occurs if the level position is closer to the center and the exchange splitting is large. An example of the calculation based on the Lorentzian state density is shown in figure 1. The results does not change much if we adopt the bell shape state density except that the secondary peak becomes more conspicuous. One can give a reasonable interpretation of the overall aspect of the wave vector dependence found by previous calculations in iron as well as in nickel with our parametrization. One might question the validity of our discussion regarding the disordered-local-moment model for nickel. In our opinion, however, the present discussion is applicable to the functional integral method employed by
Fig. 1. - The spectral densities calculated with the Lorentzian state density which simulate the calculation taking account of the short range correlation at $\Gamma_{25}$ given by reference [5]. $M$ denotes the average magnetization per atom in the unit of atomic magnetic moment; $\alpha$ is the ratio $w_{ex}/\Delta$ with $\Delta$ denoting the half-width of the Lorentzian state density; $E$ denotes the assumed position of the level measured by the distance from the center ($E = 0$) in the unit of $\Delta$. The vertical dotted lines indicates the level positions of minority and majority spins at absolute zero with $M = 1$. The abscissa is rescaled by dividing by $\alpha$ for each $\alpha$ to keep the dotted lines at the same positions.

Hasegawa [7] which utilizes CPA to take account of the magnetic disorder; although the exchange potential has there a continuous variation, its main effect may be parametrised by a value of $w_{ex}$.

We have found also that the effect of the correlation among near neighboring magnetic moments in iron discussed by Haines et al. [5] can be well reproduced by an increase of the ratio of the exchange splitting to the effective width of the band as far as the shape of the spectral density is concerned. Figure 1 shows our calculations with different values of the exchange splitting parameters which are intended to simulate the calculations of the spectral density at $\Gamma_{25}$ made by Haines et al. [5] for different choices of the degree of the correlation. If we compare our results with those given in [5], we can see a strong resemblance between the two calculations. This somewhat unexpected result suggests that it might be dangerous to deduce the degree of the short range correlation from a comparison between theory and experiment with a value of the exchange parameter fixed beforehand; for example one could determine $w_{ex}$ by fitting the calculated value of the magnetization at absolute zero to the corresponding experimental one. It is well known, however, that many body effects affect apparent values of the exchange splitting and band width in the photoemission experiment. Thus the ratio of the exchange splitting to the band width effective in determining the shape of the spectral density might be different from the value deduced from other physical quantities. It will be safer to determine all parameters including the exchange splitting and the degree of correlation with the photoemission experiment. To that purpose we will need more experimental data than those available at present. Details of the present discussions will be published elsewhere [8].