THE FORMATION OF LOCALISED MAGNETIC STATES IN ITINERANT ANTIFERROMAGNETS

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Résumé. — Les propriétés des alliages antiferromagnétiques dilués sont étudiées dans le cadre du modèle de « Anderson » pour les états magnétiques localisés. L'état fondamental du solvant s'obtient à partir d'un modèle à deux bandes de « Lomer » pour un métal antiferromagnétique itinérant (Ex. : Cr). Les fonctions de « Green » sont calculées en utilisant l'approximation « Hartree-Fock » auto-cohérente. Nous obtenons une expression analytique pour l'amplitude du moment magnétique localisé, la polarisation du spin autour de l'impureté ainsi que la variation initiale de la température de Néel en fonction de la concentration des impuretés.

Abstract. — The properties of dilute antiferromagnetic alloys are investigated in the light of Anderson's model for localised magnetic states. The host metal is described by a two-band model for itinerant antiferromagnets (Cr in particular) due to Lomer. The one-electron Green's functions for this model are obtained by the equation of motion method and a self-consistent Hartree-Fock factorisation scheme. Analytic expressions are derived for the magnitude of the localised magnetic moment, the spin polarisation near the impurity site and the initial change in Néel temperature with impurity concentration.

The ground state of antiferromagnetic chromium is a linear spin density wave (SDW) state with a single magnetic super-lattice vector **Q**. The super-lattice is incommensurate with the crystal lattice and the SDW is polarised longitudinally for temperatures $T < 120°$ and transversaly for $120° < T < T_N$ where T_N is the Néel temperature. Koehler *et al.* [1] have shown that the addition of a sufficient quantity of transition metal impurities of a higher valence than Cr yields a first order phase transition to a commensurate ground state.

In this communication we consider a single-crystal of Cr containing substitution metal impurities. The concentration of impurities is assumed sufficiently low so that (i) impurity-impurity interactions are negligible (ii) the LSDW ground state of the alloy will remain incommensurate. The electron-electron interaction which gives rise to the SDW state in pure Cr in the interband exchange interaction I of Lomer [2] and Fedders and Martin [3] between (i) electrons on the sheet of the Fermi surface centred around Γ (band I) and (ii) holes on the hole octohedron centred around H in the Brillouin zone of Cr [2] (band 2). The incommensurability is simulated by a uniaxially anisotropy field along the **Q**-vector.

The magnetic character of the impurity is described by Anderson's model [4]. The localised magnetic state is simulated by a localised non-degenerate electronic orbital at the Fermi level. The localised orbital hybridizes with both the electron hole and bands mentioned above. Localised electron of opposite spin interact via a repulsive Coulomb interaction with coupling constant I'. The one-particle Green's functions for both the conduction electrons and holes and the localised electrons are derived in the self-consistent Hartree-Fock approximation using an equation of motion method. The energy gap Δ_Q of the LSDW state is then written :

$$\Delta_Q = -\frac{I}{2}\sum_{k,\sigma}\sigma < a_{k\sigma}^{(1)+}\, a_{k+Q\sigma}^{(2)} > \qquad (1)$$

where $a_{k\sigma}^{(i)+}\, a_{(k\sigma}^{(i)})$ creates (destroys) an electron in band i ($i = 1,2$). The thermodynamics average in (1) describes triplet interband electron-hole pairs separated by a wave vector **Q**. The formation of such pairs for temperatures $T < T_N$ gives rise to an antiferromagnetic LSDW with wave vector **Q**. The magnitude of the localised moment on the impurity site is described by the parameter Δ_l defined as :

$$\Delta_l = -\frac{I'}{2}\sum_{\sigma}\sigma < A_\sigma^+\, A_\sigma > \qquad (2)$$

$A_\sigma^+(A_\sigma)$ creates (destroys) an electron of spin σ in a localised impurity state. The Hartree-Fock analysis yields a set of self-consistent equations relating Δ_l and Δ_Q. In the limit of dilute impurity concentration and zero temperature Δ_l is given by the integral equation :

$$\Delta_l = -\left(1 - I'\, J_1(\Delta_Q^{(0)}, \Delta_l)\right)^{-1} \times \text{where} \qquad \times I'\, \Gamma_{cr}\, J_2(\Delta_Q^{(0)}, \Delta_l) \qquad (3)$$

$$J_i(\Delta_q^{(0)}\Delta_l) = \frac{1}{\pi}\int_0^\infty \frac{d\omega(\omega^2 + \Delta_Q^{(0)2})^{n_i}}{\left[(\omega^2+\Delta_Q^{(0)2})^{1/2}+\Gamma^+\right]^2\omega^2 + \left[\Delta_l(\omega^2+\Delta_Q^{(0)2})^{1/2} - \Gamma_{cr}\,\Delta_Q^{(0)}\right]^2} \qquad (4)$$

and $n_1 = 1$; $n_2 = \frac{1}{2}$. Γ^+ is the width of the localised electronic level in a two-band model and Γ_{cr} is the width of a localised triplet particle-hole pair due to the hybredizing interaction. In general $\Gamma^+ \geqslant \sqrt{2}\Gamma_{cr}$. $\Delta_q^{(o)}$ is the energy gap of the pure antiferromagnet. (3) has been solved numerically for Δ_l and the result is show in figure 1 for fixed values of the parameters. Let $\Delta_l^{(0)}$ be the magnetic moment in the absence of the LSDW ground state. Then $\Delta_l^{(0)} \neq 0$ only when $I' > \sigma\Gamma^+$ (see Fig. 1 and reference [4]). For each value of I' satisfying this condition, there are two solutions for $\Delta_l^{(0)}$ of equal magnitude and opposite sign indicating that the direction of the local moment is arbitrary. The introduction of the LSDW ground state in the host metal also gives rise to two solutions for Δ_l. However one of these solutions is physically unacceptable. (See Fig. 1.) The other solution yields a non-zero value of Δ_l for all finite values of I', both positive and negative. When $I' \gg \pi\Gamma^+$, $\Delta_l \approx -|\Delta_l^{(0)}|$ i. e. the magnetic moment is alligned anti-parallel to

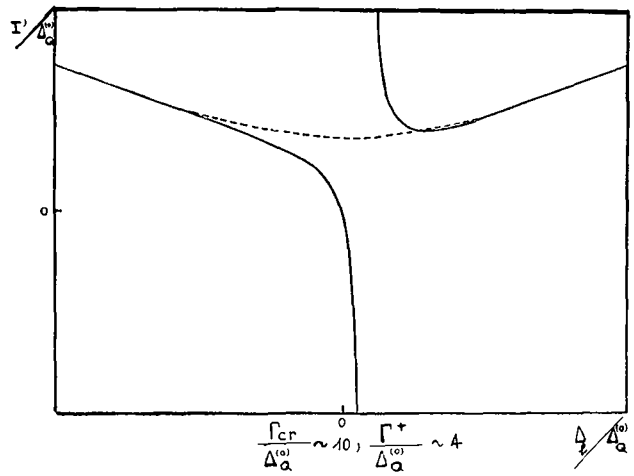

FIG. 1. — The localised magnetic moment Δ_l as a function of I'. The dotted curve gives Δ_l in the absence of antiferromagnetism — the solid curve on the left of the figure exhibits Δ_l for an antiferromagnetic alloy. The solid curve on the right of the figure corresponds to a physically unacceptable solution.

the direction of the LSDW at the impurity site. When $I' < 0$, Δ_l becomes positive and saturates as $I' \to -\infty$. The reason for the saturation is that Δ_l is a function of

$$I'_{\text{eff}} = I'(1 - I'/\pi\Gamma)^{-1} \quad \text{for} \quad I' < 0 .$$

Negative values of I' are allowable if I' is interpreted as the change in the interband interaction I of the host lattice at the impurity site [5].

The change in electron spin polarisation at the impurity site due to the local moment is given by :

$$\delta\sigma(\mathbf{R}) = -\frac{4\,\Gamma_{cr}}{\pi N(0)\,(\Gamma^{+2} + \Delta_l^2)} \left(\frac{m^*}{4\,\pi R}\right) \times$$
$$\times \left\{ |\,\Delta_l^{(0)}\,|\,\Delta_Q^{(0)}\,K_1\left(\frac{2\,R}{\xi}\right)\cos(2\,k_F\,R) + \right.$$
$$\left. + \Gamma^+\,\Delta_Q^{(0)}\,K_0\left(\frac{2\,R}{\xi}\right)[1 - \cos(2\,k_F\,R)] \right\} \qquad (5)$$

when $I' \gg \pi\Gamma^+$. $K_0(x)$ and $K_1(x)$ are modified Bessel functions, R is the distance from the impurity site, ξ is the coherence length of host antiferromagnet and k_F is the Fermi momentum. Equation (5) shows that the RKKY oscillations in the spin polarisation are completely suppressed for distances $R > \xi$.

The initial change in Néel temperature with impurity concentration n_I can now be written [6] :

$$\left.\frac{\partial T_N}{\partial n_I}\right|_{n_I=0} \approx -\frac{1}{k}\left\{\frac{\pi h}{4\,\tau_{NM}} + \frac{1}{N(0)}\left(\frac{1}{2} - \frac{\Gamma_{cr}^2}{\Gamma^{+2}}\right)\right\} +$$
$$+ \frac{T_{N0}\,I'_{\text{eff}}\,\Gamma_{cr}^2}{\pi I'^{+2}} \ln^2\left(\frac{2\,\gamma_e\,\Gamma^+}{\pi k T_{N0}}\right) + \left(\frac{\partial T_N}{\partial n_I}\right)_{D,S}, \qquad (6)$$

$N(0)$ is the paramagnetic density of states of conduction electrons at the Fermi level, τ_{NM} is the relaxation time of the conduction electrons due to potential scattering by the impurities, T_{N0} is the Néel temperature of the pure metal and γ_e is Euler's constant. The effect of τ_{NM} on T_N has been investigated by Zittartz [7]. The first term on the right hand side of (6) indicates that resonance scattering enhances the effect of potential scattering on T_N. The second term may be positive or negative depending on the sign of I' and becomes singular at the Anderson criterion for the formation of a localised moment in the absence of antiferromagnetism. $(\delta T_N/\delta n_I)_{D.S.}$ is the change in Néel temperature due to the change in electronic density of states of the host metal by the impurity. For transition metal impurities in Cr, all these terms are important and it is difficult to make a qualitative comparison with experiment.

Work is in progress to investigate the geometrical implication and the spin dynamics of this metal.

Acknowledgements. — The author wishes to thank Professors L.-M. Falicov, P.-R. Wallace and A. Caillé for stimulating discussions and Dr G. Morandi for interesting correspondance.

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