Magnetism of impurities in Hume-Rothery metallic phases

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It is stressed that the variations of the density of states near the Fermi level in Hume-Rothery phases should not alter much the condition of appearance of magnetism in transitional impurities, compared with their behaviour in normal metals of similar electron per atom ratio. The cases of a lanthanide such as Ce in normal metals or of transitional metals in a semimetal such as Bi would be different.

I. Introduction

The coherent scattering of valence electrons on the atomic structure of Hume Rothery Jones metallic phases introduces a specific feature in the density of states $n(E)$ near the Fermi level. This is responsible for their relative çtability witli respect to other structures.

The possible magnetism of transitional impurities in normal metals, with nearly free valence electrons, is related to the ratio of the exchange energy to tlie resonance broadening of the d shell with the valence electrons. For a slowly varying density of states, tlie broadening is proportional to it.

One could then expect large variations of magnetism for these impiirities when dissolved in Hume Rothery phases compared to other phases.

II. Density of states in a Hume Rothery metallic phase

If the scattering potential $v(k)$ responsible for tlie Hume Rothery Jones diffraction is treated within simple first order (kinematic) perturbation, its introduction shifts the energy E_k^0 of a $|k>$ state to

$$E_k = E_k^0 + \frac{|v(k)|^2}{E_k^0 - E_{k-K}^0} \qquad (1)$$

A classical development then shows that, within this approximation, the density of states $n(E)$ tends to ∞ or $-\infty$ below and above the critica1 energy

$$E_k^0 = E_{k-K}^0 = E_{1/2K}^0 \qquad (2)$$

A more correct two waves (dynamical) analysis of tlie diffraction shows that this very strong anomaly is replaced by two sucessive 3d van Hove anomalies, i. e. a finite peak of n(E) followed by a finite angle of $n(E)$, each one with a cliange of slope. These anomalies are separated by a band gap $2|v(\kappa)|$, on either side of $E_{1/2\,\kappa}^0$. In this approach as in the rougher one above, the whole of the density anomaly extends over an effective width of a few $|v(\kappa)|$.

III. Resonance broadening of an impurity

In normal metals where the density of states $n^0(E)$ varies slowly with E near the Fermi level the resonance broadening of a transitional impurity is of the order

$$w^0 = |V_{kd}|^2 n^0(E_M) \,, \qquad (3)$$

where v_{kd} is the coupling potential between the d states and the metallic k states.

If the density of states $n(E)$ of Hume Rothery phases varied slowly enough'with energy E, one should expect a similar relation between the broadening w and $n(E)$:

$$w = |\nu_{kd}|^2 n(E_M) \,. \qquad (4)$$

Now, for Huine Rothery phases, tlie inaximum stability occurs when E_M is near a miniinum of $n(E)$. One could then expect tlie broadening w of tlie d state to be smaller, thus sucli impurities bave show a stronger tendency to show a large magnetic moineiit at high temperatures and a correlative Kondo effect at low ones.

But in fact, for "normal" metals such as Cu, Zn, Al, wliere deviations froin free electron behaviour are weak, $|v(k)|$.is small, typically of order of a small fraction of e.v., w is on the other hancl of order or larger tliaii 1 eV. In sucli conditioiis, tlie preceeding analysis is no longer valicl, as the kd mixing affects of tlie whole width of tlie van Hove anomaly. Tlie magnetic behaviour of transitional impurities will then be little affected by the special character of tlie Hume Rothery phases.

Similar meclianisms probably hold for actinides in normal metals, where tlie mixing potential v_{kf} is again large. Indeecl tlie only cases where the anomaly discussed here could shom up strongly are these of resonating f sliells of lanthanides sucli as Cerium, where $|v_{kf}|$ is much weaker than $|v_{kd}|$, or transition iinpurities in semi metals such as bismutli, wliere $|v_k|$ is large.