TWO NEARLY MAGNETIC IMPURITIES IN NON-MAGNETIC HOST

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Two Anderson-like impurities are considered. If an isolated impurity is assumed to be nearly magnetic then we find that each of the two impurities can be magnetic, nonmagnetic or nearly magnetic, depending on the distance between them. The relation to PdNi alloys is briefly discussed.

1. *Formulation and results*

The Anderson model of an impurity in a non-magnetic host is very useful for describing the situation which takes place in dilute paramagnetic alloys ([1, 2] and references cited therein). An Anderson-like impurity may carry the magnetic moment or not, depending on the relation between the values of its energy level E, intraatomic Coulomb interaction parameter I, the density of states of the host electrons ϱ and the mixing potential between host and impurity electrons V. Let us consider two identical impurities localized in $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$. If one denotes the host band energy function by ε_k and takes into account the above remarks then the second-quantized form of the Hamiltonian reads

$$H = \sum_{k,\alpha} \varepsilon_k c^+_{k\alpha} c_{k\alpha} + E \sum_{i=1}^{2} d^+_{i\alpha} d_{i\alpha} + I \sum_{i=1}^{2} d^+_{i\uparrow} d_{i\uparrow} d^+_{i\downarrow} d_{i\downarrow}$$

$$+ \frac{V}{\sqrt{N}} \sum_{k,\alpha} \sum_{i=1}^{2} (e^{-ik\cdot r_i} c^+_{k\alpha} d_{i\alpha} + e^{ik\cdot r_i} d^+_{i\alpha} c_{k\alpha}), \tag{1}$$

where $i, j = 1, 2$ and $i \neq j$. It must be stressed that we do not assume any form of the direct interaction between impurities.

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Using the well-known method of equations of motion for the Fourier-transformed double time Green functions (see [3] for details) it is easy to find from (1) in the Hartree-Fock approximation

$$(\omega - E_\alpha)\langle\langle d_{i\alpha}|d_{i\alpha}^+\rangle\rangle = 1 + \frac{V}{\sqrt{N}}\sum_k e^{ik\cdot r_i}\langle\langle c_{k\alpha}|d_{i\alpha}^+\rangle\rangle$$

$$(\omega - \varepsilon_k)\langle\langle c_{k\alpha}|d_{i\alpha}^+\rangle\rangle = \frac{V}{\sqrt{N}}\sum_{l=1}^{2} e^{-ik\cdot r_l}\langle\langle d_{l\alpha}|d_{i\alpha}^+\rangle\rangle$$

$$(\omega - E_\alpha)\langle\langle d_{j\alpha}|d_{i\alpha}^+\rangle\rangle = \frac{V}{\sqrt{N}}\sum_k e^{ik\cdot r_j}\langle\langle c_{k\alpha}|d_{i\alpha}^+\rangle\rangle. \tag{2}$$

System (2) can be solved with respect to $\langle\langle d_{i\alpha}|d_{i\alpha}^+\rangle\rangle$. Let us assume for simplicity that $\boldsymbol{r}_1 = 0$, $\boldsymbol{r}_2 = \boldsymbol{a}$. Since the impurities are identical we can drop the index "i". We get

$$\langle\langle d_\alpha|d_\alpha^+\rangle\rangle = (\omega - E_\alpha - M(\omega))^{-1}, \tag{3}$$

where

$$E_\alpha = E + I\langle n_{-\alpha}^d\rangle, \quad \langle n_\alpha^d\rangle \equiv \langle d_\alpha^+ d_\alpha\rangle$$

$$M(\omega) = V^2\{F(\omega) + V^2 F_+(\omega)F_-(\omega)\,[\omega - E_\alpha - V^2F(\omega)]^{-1}\}$$

$$F(\omega) = \frac{1}{N}\sum_k \frac{1}{\omega - \varepsilon_k}, \quad F_\pm(\omega) = \frac{1}{N}\sum_k \frac{\exp(\pm ik\cdot a)}{\omega - \varepsilon_k}.$$

$\langle\ldots\rangle$ stands for the thermal average. For our qualitative considerations it is enough to consider the case $M(\omega) \simeq M(0)$ i.e. approximate the self-energy term by its value at the Fermi level [2]. For the Lorentzian density of states function it can be assumed $F(\omega) \simeq -i\pi\varrho$ and for $F_\pm(\omega)$ [4]

$$F_\pm(\omega) = -\frac{\pi\varrho(0)}{\beta}e^{i\beta}$$

where $\beta = k_F a$. The latter relation is reasonable for $\beta > 1$. $\langle n_\alpha^d\rangle$ is simply related to $\langle\langle d_\alpha|d_\alpha^+\rangle\rangle$ $(T = 0)$

$$\langle n_\alpha^d\rangle = \int_{-\infty}^{0}\left(-\frac{1}{\pi}\,\mathrm{Im}\,\langle\langle d_\alpha|d_\alpha^+\rangle\rangle\right)d\omega,$$

and we get after some manipulations

$$\langle n_\alpha^d\rangle = \frac{1}{\pi}\,\mathrm{ctg}^{-1}\left[\frac{E_\alpha + \dfrac{b^2}{\beta^2}\,\dfrac{b\sin 2\beta - E_\alpha\cos 2\beta}{E_\alpha^2 + b^2}}{b + \dfrac{b^2}{\beta^2}\,\dfrac{E_\alpha\sin 2\beta + b\cos 2\beta}{E_\alpha^2 + b^2}}\right], \tag{4}$$

where $b = \pi\varrho V^2$.

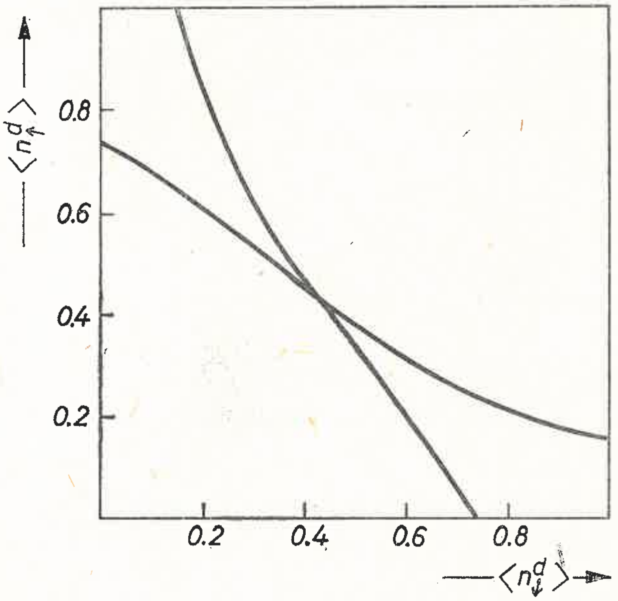

Fig. 1. An isolated impurity, $\beta \to \infty$

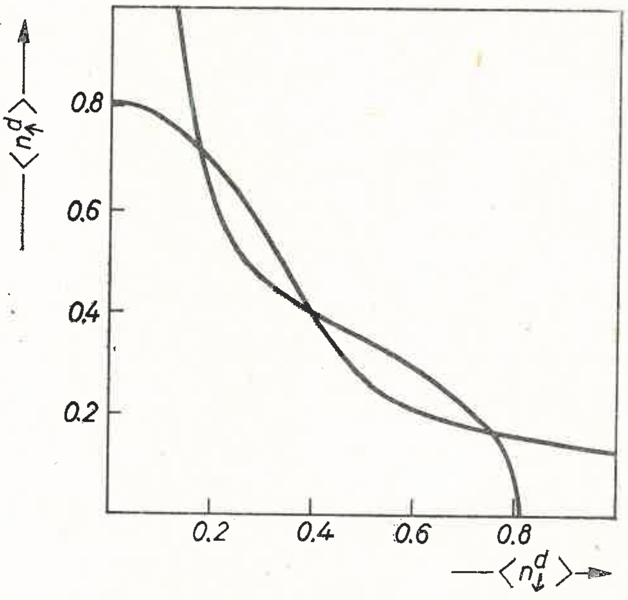

Fig. 2. Two impurities, $\beta = 1.6$

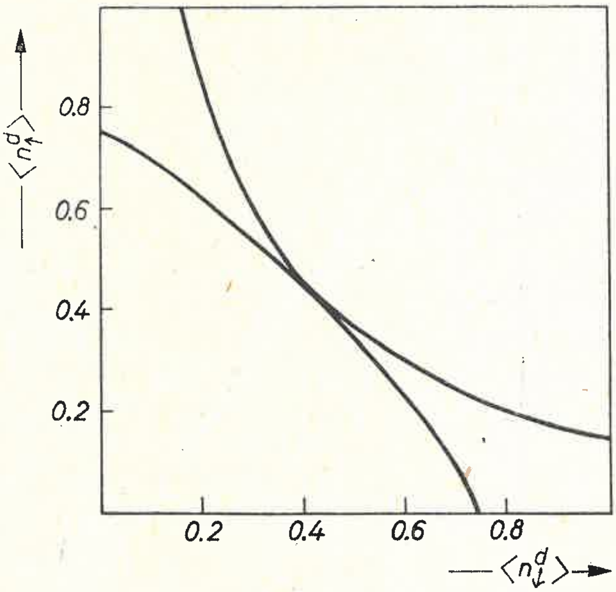

Fig. 3. Two impurities, $\beta = 3.1$

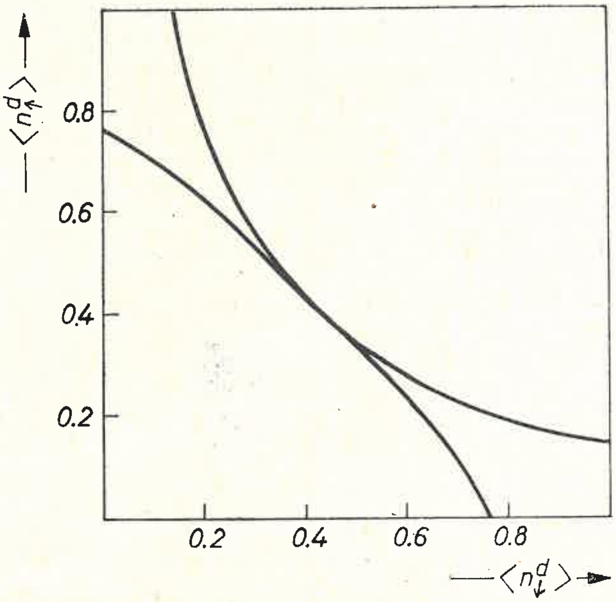

Fig. 4. Two impurities, $\beta = 4.6$

The case $\beta \to \infty$ corresponds to an isolated impurity. The set of equations (4) can be solved graphically and this is presented in figures 1–4 for $\beta \to \infty$, $\beta = 1.6$, 3.1 and 4.6 respectively.

2. *Discussion*

Fig. 1 corresponds to the case of an isolated impurity which is nearly magnetic. The values of the parameters are: $E = -0.4$ eV, $I = 1.2$ eV. $b = 0.4$ eV and it may be checked that for $b = 0.3$ eV the well-defined magnetic solutions exist. For $\beta = 1.6$ the magnetic moment appears (Fig. 2) but for $\beta = 3.1$ (Fig. 3) each of the impurities is more distant from magnetic instability than an isolated impurity (compare Fig. 3 and Fig. 1). If we increase the distance to $\beta = 4.6$ then each impurity falls into a state which is more instable with respect to magnetism than that of an isolated one (Fig. 4). Before we shall try to draw any conclusions, let us mention that all these effects will be completely invisible if the state of a single impurity is not so close to magnetic instability. This may be checked for e.g. $b = 0.5$ eV.

The conclusion which may be drawn is that the formation of complex clusters is not necessary for magnetic moments to appear, provided that an isolated impurity is close enough to magnetic instability.

The explanation of experimental results for dilute paramagnetic P<u>d</u>Ni alloys is possible only if one assumes that at least a part of Ni atoms carries a well-defined moment (see [5] and references cited therein). Ni atoms, when dissolved in palladium, nearly satisfy the local moment formation criterion [6] and if one treats the Ni atoms as carrying the well-defined magnetic moments then one can get reasonable results for temperature dependence of magnetic susceptibility of dilute P<u>d</u>Ni alloys [7]. Certainly, the above results may serve only to get some physical intuition (HF approximation is not valid in the magnetic region [8]). Also the applicability of the Anderson model for Ni when dissolved in palladium is not quite evident. This is due to the fact that one should take into account the exchange interaction between host electrons. However, for our qualitative discussion it may be contained implicitly in ϱ. The calculations in which the host electrons are interacting are under way and will be published.

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