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LOCAL ENVIRONMENT EFFECT IN ALLOY MAGNETIZATION

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Résumé. — L’effet de l’environnement local sur le comportement magnétique d’une impureté dans un métal, suggéré pour la première fois par Jaccarino et Walker est étudié par un modèle d’Anderson étendu au cas d’impuretés multiples. On explique cet effet par le fait que la susceptibilité de l’impureté dépend de la distribution des autres impuretés dans son entourage.

Abstract. — The local environment effect in the magnetic behavior of an impurity in a metal first suggested by Jaccarino and Walker is studied on the basis of the Anderson model extended to the many impurity case. The local environment effect is understood from the fact that the magnetic susceptibility of an impurity depends on the distribution of other impurities in its neighborhood.

Since the work of Friedel, Anderson and Wolff the occurrence or non-occurrence of a local magnetic moment on an impurity in a metal was understood in close correlation with the bulk properties of the host metal such as the density of states at the Fermi surface. Later in 1965, however, Jaccarino and Walker [1, 2] presented a counter viewpoint based on the analysis of Co Knight shift in RhPd host. Jaccarino and Walker suggested that the occurrence or non-occurrence of a localized moment on an impurity is determined mainly by the number of other surrounding impurities in its immediate vicinity rather than the bulk properties of the host metals. This local environment effect has been seen in a number of other alloys [3].

In this paper we present a simple discussion on the possible mechanisms for the local environment effect based on the Anderson model extended to the many impurity case [4]. By using the two-time Green’s function we calculate the self-energy of an impurity due to its interaction with the other surrounding impurities. The real and imaginary parts of the self-energy give rise, respectively, to the shift and the broadening (or narrowing) of the impurity state. The local environment effects originate from the fact that the self-energy of an impurity depends on the distribution of other impurities in its immediate neighborhood. We show this by calculating the magnetic susceptibility of the impurity.

We assume the impurity levels are not orbitally degenerate and the host metal is represented by a free electron band. Then the Green’s function of the i\textsuperscript{th} impurity case \( G_{i\pm}(\omega) \) is calculated in the Hartree-Fock approximation:

\[
G_{i\pm}(\omega) = \frac{1}{\omega - E^0_{i\pm} - U_i N_{i\pm} - V_i F_{o\pm}(\omega) - \Sigma_{i\pm}(\omega)}
\]

\[
\Sigma_{i\pm}(\omega) = \sum_{j \neq i} (V_j V_j F_{ij\pm}(\omega) + T_{ij}) \times \frac{G_{j\pm}(\omega)}{\omega - E^0_{j\pm}} (V_j V_j F_{jj\pm}(\omega) + T_{jj})
\]  

(1)

In eq. (1), \( E^0_{i\pm} = E^0_i \pm \mu H \), where \( E^0_i \) is the unperturbed energy level of the \( i \)\textsuperscript{th} impurity and \( \pm \mu H \) is the Zeeman energy due to the external magnetic field \( H \) along the \( z \) axis, \( U_i \) is the Coulomb repulsion at the \( i \)\textsuperscript{th} impurity site, \( N_{i\pm} \) is the expectation value of the number of localized electrons at the \( i \)\textsuperscript{th} impurity, \( V_i \) is the matrix element of the s-d mixing of the \( i \)\textsuperscript{th} impurity with the host metal conduction band which we assume to be real and

\[
F_{o\pm}(\omega) = \frac{\omega - \varepsilon_{e\pm} + i \eta^+}{\omega - \varepsilon_{e\pm} + i \eta^{-}}
\]

where \( \varepsilon_{e\pm} = \varepsilon_e \pm \mu H \) is the energy of a conduction electron with wave number \( k \) including the Zeeman energy, \( \rho_{e\pm}(\omega) \) which is obtained from the imaginary part of \( F_{o\pm}(\omega) \) is the unperturbed density of states of the host metal conduction electrons. Notice if the species of all impurities are the same, we can drop the suffixes \( e\pm \) from \( E^0_i, U_i \) and \( V_i \). Also when we refer to a quantity without the external magnetic field (and at the paramagnetic state) we can drop the spin suffixes \( \pm \). The self-energy due to the interaction with other impurities, \( \Sigma_{i\pm}(\omega) \), is given by eq. (2). The difference between \( G_{i\pm}(\omega) \) and the single impurity limit Green’s function \( G_{i\pm}(\omega) \), is just this self-energy term.

In eq. (2), \( T_{ij} \) is the direct transfer energy between the \( i \)\textsuperscript{th} and \( j \)\textsuperscript{th} impurities and

\[
F_{ij\pm}(\omega) = \sum_k \exp[ik(R_i - R_j)] \left( \omega - \varepsilon_{e\pm} + i \eta^{-} \right)^{-1}
\]

For a parabolic band

\[
F_{g}(\omega) = - \Omega/4 \pi^2 m/\hbar^2 \times \frac{1}{R} \exp[i \{ 2 m/\hbar^2 (\omega - \varepsilon_e) \}^{1/2} R]
\]

where \( \Omega \) is the volume of the system, \( m \) is the mass of a conduction electron and \( \varepsilon_e \) is the bottom of the conduction band.

A Green’s function of the form of eq. (1) was used earlier to discuss the effective exchange interaction between localized moments [5]. In these earlier works[5], however, the occurrence of a local moment was assumed from the beginning. In this paper the magnetic susceptibility of the individual impurity states is calculated from \( G_{o}(\omega) \) by assuming the impurity state does not form a local moment. The magnetic susceptibility of the \( i \)\textsuperscript{th} impurity, \( \chi_i \) is defined in terms of the expectation value of the number of electrons at the impurity

\[
N_{i\pm} = N_i \mp \Delta N_i
\]

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as \[ \chi_i = \mu (N_i - N_{i+})/H = 2 \mu \Delta N_i/H, \]
where \( N_{i\pm} \) is obtained from the imaginary part of
\[ G_{i\pm}(\omega) : N_{i\pm} = -\frac{1}{\pi} \int_{-\infty}^{\infty} d\omega f(\omega) \text{Im} G_{i\pm}(\omega), \]
and \( f(\omega) \) is the Fermi distribution function.

To make the calculation of \( N_{i\pm} \) feasible, we neglect the \( \omega \) dependence of the last two terms in the bracket of eq. (1) by replacing \( \omega \) with the chemical potential which we choose as the zero of measuring energy. In this approximation the density of states of an impurity becomes a Lorentzian:
\[ G_{i\pm}(\omega) = \left[ (\omega - E_{i\pm}) + i\Delta_i \right]^{-1} \]
with the width of the impurity state is given as
\[ \Delta_i = \Delta_i^0 + \delta\Delta_i, \]
where \( \Delta_i^0 \) is the familiar single impurity limit width of the impurity state, \( nV_i^2 \rho_i^0(0) \), and \( \delta\Delta_i \) is the modification of the width due to the presence of other impurities:
\[ \delta\Delta_i = -\text{Im} \Sigma(0). \]

Notice that the magnetic field dependence of the width does not come into the calculation of the linear susceptibility and is therefore neglected. Similarly the energy level of the impurity state is given as
\[ E_i = E_0 + U_i N_i + V_i^2 \rho_i^0(0) + \text{Re} \Sigma(0) \]
where
\[ \Delta E_i = \mu H + U_i \Delta N_i + \sum_{j(\neq i)} c_{ij} U_j \Delta N_j, \]
and the coupling constant, \( c_{ij} \), of the effective exchange interaction between impurities is given as
\[ U_j c_{ij} = \text{Re} \left[ (V_i V_j F_{ij}(0) + T_{ij})^2 \frac{\partial}{\partial N_j} G_j^0(0) \right]. \]

A more detailed discussion about \( \delta\Delta_i \) and \( c_{ij} \) is given in Ref. [4].

The possible origins of the local environment effect can be catalogued as being due to the impurity site dependence of the following effects. (Ia) \( \delta\Delta_i \): the broadening or narrowing of the impurity level, (Ib) \( \text{Re} \Sigma(0) \): the shifting of the impurity level, (II) \[ \sum_{j(\neq i)} c_{ij} U_j \Delta N_j \]: the exchange interaction between impurities. The effects of (Ia) and (Ib) modify the impurity density of states from \( \rho_i^0(0) = -1/\pi \text{Im} G_i(0) \) to \( \rho_i(0) = -1/\pi \text{Im} G_i(0) \). The effect of (II) can be seen from the following coupled equations between the impurities susceptibilities
\[ \chi_i = \chi_i^0 + \frac{1}{2\mu^2} \sum_{j(\neq i)} c_{ij} U_j \chi_j, \]
where \( \chi_i^0 = 2 \mu^2 \rho_i(0)/1 - U_i \rho_i(0) \) and we used the low temperature limit approximation. The effects of (Ia) and (Ib) are included in \( \chi_i^0 \). In \( \chi_i^0 \) the modified impurity density of states \( \rho_i(0) \) appears whereas in the single impurity limit susceptibility, \( \chi_i^{00} \), \( \rho_i^0(0) \) appears:
\[ \chi_i^{00} = 2 \mu^2 \rho_i^0(0)/1 - U_i \rho_i^0(0). \]

In this case the exchange interaction between impurities, effect (II), seems to be playing an important role. We consider a cluster of nickel atoms, in which a central nickel atom is surrounded by \( z \) other nickel atoms at its nearest neighbor sites. We assume the exchange interaction is only between the central nickel atom and its nearest neighbor nickel atoms with coupling constant \( c_{01} \). Then the coupled equation (7) for this cluster is solved to give
\[ \chi_0 = \frac{1}{C. D.} \left[ \chi_0^0 + z c_{01} \left( \frac{1}{2\mu^2} U \chi_0^0 \chi_1 \right) \right], \]
\[ \chi_1 = \frac{1}{C. D.} \left[ \chi_1^0 + c_{01} \left( \frac{1}{2\mu^2} U \chi_0^0 \chi_1 \right) \right], \]
where the common denominator is given by
\[ C. D. \equiv 1 - z^2 c_{01} \left( \frac{1}{2\mu^2} U \chi_0^0 \right) \left( \frac{1}{2\mu^2} U \chi_1^0 \right). \]

Notice the difference between the susceptibilities of a central nickel atom and the surrounding nickel atoms, \( \chi_0 \) and \( \chi_1 \), is the numerator. The denominator is the same. Namely the «Curie point» is the same but the «Curie constants» which give the magnitudes of the local moments are different. As discussed in Ref. [4] the coupling constant \( c_{01} \) is on the order of 1 and \( (1/2\mu^2) U \chi_0^0 \) or \( (1/2\mu^2) U \chi_1^0 \) is on the order of the exchange enhancement factor of the impurity. In the present case of nickel in copper with the nickel enhancement factor bigger than 1 we can easily conceive of a situation where \( \chi_0 > \chi_1 > \chi_0^{00} \) even if \( \rho_0(0) < \rho_1(0) < \rho_0^0(0) \) for \( z > 10 \).

References

[3] For references see Ref. [4].