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CONTRIBUTION TO THE THEORY OF INVAR ALLOYS

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One of us, together with Sedov, has shown in [1] that the anomalies of invar alloys can be explained by assuming that an exchange interaction that disrupts in part the parallel spin orientation exists between the electrons of neighboring iron ions in the face-centered lattice of these alloys. That is to say, the exchange integral is negative for neighboring iron ions, $I^{FeFe} < 0$, whereas the corresonding integrals I^{FeNi} and I^{NiNi} are positive. The model proposed in [1] was further devloped in [2, 3]. The features of invar alloys were discussed recently also from the point of view of the model of rigid bands in [4, 5].

The main shorcoming of [1 - 3] was that the localized-spin model used in them was more readily suitable for dielectrics than for metallic alloys. The shortcoming of [4, 5], to the contrary, was that they were based on a model in which no account was taken of the singularities of the state-density curve for a disordered alloy. Nor was allowance made for the exchange interaction between nearest neighbors, which strongly influences the magnetic properties of alloys [6, 7].

In the present article we discuss the properties of invar alloys from the point of view of the model of strongly coupled electron and we use the coherent potential method (CPA) proposed by Soven [8] and by Velicky et al [9] (see also [10]). We introduce in the Hamiltonian additional parameters that characterize the electron exchange interaction between neighboring ions, averaged over the configurations.

We express the Hamiltonian for a binary ferromagnetic alloy in the form

$$H = H_1 + H_2, \tag{1}$$

$$H_1 = \sum_{n,m\sigma} t_{nm} a^+_{n\sigma} a_{m\sigma} + \sum_{n,\sigma} \epsilon_n n_{n\sigma} + (1/2) \sum_{n,\sigma} U_n n_{n\sigma} n_{n,-\sigma}, \tag{2}$$

$$H_2 = -2 \sum_{n,m} I_{nm} (S^x_n S^x_m + S^y_n S^y_m + S^z_n S^z_m), \tag{3}$$

$$\begin{aligned} S^x_n &= (1/2)(a^+_{n\uparrow} a_{n\downarrow} + a^+_{n\downarrow} a_{n\uparrow}), \\ S^y_n &= (1/2i)(a^+_{n\uparrow} a_{n\downarrow} - a^+_{n\downarrow} a_{n\uparrow}), \\ S^z_n &= (1/2)(n_{n\uparrow} - n_{n\downarrow}), \end{aligned} \tag{4}$$

where $t_{nm} = t^{AA}_{nm}$, t^{AB}_{nm}, t^{AB}_{nm} are the transfer integrals and $I_{nm} = I^{AA}$, I^{AB}, and I^{BB} are the exchange integrals between the electrons of the nearest-neighbor ions A and B occupying lattice points n and m, $\epsilon_n = \epsilon^A$, ϵ^B, $U_n = U^A$, U^B are integrals characterizing the Coulomb interaction of the electrons at the ions of kind A and B occupying the site n, and $a^+_{n\sigma}$ and $a_{n\sigma}$ are the creation and annihilation operators for electrons with spin σ at the site n. We associate with each site two states, one with spin up and the other with spin down. In the considered case of invar alloys we assume, as in [1], that $I^{AA} < 0$, $I^{AB} > 0$, $I^{BB} > 0$ and $U^A = U^B = U$.

We seek a solution for the average energy and the average magnetic moments in the Hartree-Fock approximation, replacing in the third sum of the Hamiltonian H_1 the operator $n_{n,-\sigma}$ by its

mean value $\langle n_{n,-\sigma} \rangle$ and representing H_2 in the form

$$H_2 = -\sum_{n,m,\sigma} I_{nm}\, a^+_{n\sigma}\, a_{n,-\sigma}\, a^+_{m,-\sigma}\, a_{m\sigma} - (z/2) \sum_n I_n (n_{n\uparrow} - n_{n\downarrow}), \tag{5}$$

where

$$I_n = I^A, I^B,$$

$$I^A = x I^{AA} M_A + y I^{AB} M_B, \tag{6}$$

$$I^B = x I^{AB} M_A + y I^{BB} M_B$$

z is the number of nearest neighbors (z = 12 in our case), x and y are the concentrations of ions of kind A and B, respectively, and M_A and M_B are the average magnetic moments expressed in Bohr magnetons, $M_{A(B)} = \langle n^{A(B)}_{n\uparrow} \rangle - \langle n^{A(B)}_{n\downarrow} \rangle^A$.

In our case we disregard differences of the type $t^{AA}_{nm} - t^{BB}_{nm}$, and put

$$t^{AA}_{nm} = t^{AB}_{nm} = t^{BB}_{nm} = t^{(0)}_{nm}. \tag{7}$$

Substituting (5) in (1), neglecting in (5) the first sum, which is small at low temperatures in comparison with the second, taking (7) into account, and introducing the mean value $\langle n_{n,-\sigma} \rangle$, we express the Hamiltonian in the form

$$H = \sum_\alpha H_\sigma = \sum_{n,m,\sigma} t^{(0)}_{nm}\, a^+_{n\sigma}\, a_{m\sigma} + (1/2) \sum_{n\sigma} \epsilon_{n\sigma}\, n_{n\sigma}, \tag{8}$$

where

$$\epsilon_{n\uparrow} = \epsilon^{A(B)}_{\uparrow} = \epsilon^{A(B)} + (1/2)\,[U \langle n^{A(B)}_{n,-\sigma} \rangle - z I^{A(B)}],$$

$$\epsilon_{n\downarrow} = \epsilon^{A(B)}_{\downarrow} = \epsilon^{A(B)} + (1/2)\,[U \langle n^{A(B)}_{n\sigma} \rangle + z I^{A(B)}]. \tag{9}$$

With a Hamiltonian of this type we can use the CPA procedure.

We have calculated the average atomic moments of the components of a disordered alloy under various assumptions concerning the shape of the state-density curve. We present here the calculation results for two limiting cases: 1) the case of split narrow bands, when $\delta_\sigma \gg 1$, and 2) the case of a pseudocrystal, when, to the contrary, $\delta_\sigma \ll 1$, where $\delta_\sigma = \epsilon^A - \epsilon^B/W$ and W is the width of the band. The case of an insulator, when W = 0, is excluded in this case, i.e., for $\delta_\sigma \gg 1$ and $W \to 0$ we consider the limiting case when the self-consistent-field method is still valid.

In the first case, as $W \to 0$, the calculation leads to the following expressions for the atomic magnetic moments

$$M_A = n^A_0, \; M_B = n^B_0 \qquad \text{if} \quad x \leqslant x_0, \tag{10a}$$

$$M_A = \frac{(1-x) I^{AB}}{x |I^{AA}| - (U/2z)}\, n^B_0 \qquad \text{if} \quad x \geqslant x_0, \tag{10b}$$

$$x_0 = 1 + \frac{1}{2z} \frac{U}{I^{AB}} \frac{n^A_0}{n^B_0} \Big/ 1 + \frac{|I^{AA}|}{I^{AB}} \frac{n^A_0}{n^B_0} \tag{11}$$

n^A_0 and n^B_0 are the numbers of electrons per atom in the pure metal A or B, respectively. Formulas (10) describe qualitatively correctly the observed concentration dependence of the average magnetic moments $M = xM_{Fe} + yM_{Ni}$ of the alloys. By specifying I and U/z we can roughly estimate the concnetration x_0. Thus, at $|I^{AA}| \simeq I^{AB} \simeq I^{BB} \simeq U/z$, substituting $n^A_0 - n^{Fe}_0 = 2.6$ and $n^B_0 = n^{Ni}_0 = 0.6$, we obtain from (11) $x_0 \simeq 0.6$, which agrees with the observed value.

In the case of a pseudocrystal and bands of rectangular shape, the calculation leads to the expression

$$M = xM_A + yM_B = (\nu / 2WN)\{xM_A[(U/2z) + xI^{AA} + yI^{AB}] + \\ + yM_B[(U/2z) + xI^{AB} + yI^{BB}]\}, \quad (12)$$

where ν is the number of states in the band and N is the number of atoms of the alloy.

Since $\delta_\sigma << 1$ in our case, which is equivalent to W >> U, I, the equalities in (12) are compatible only if $M = M_A = M_B = 0$. The limiting case of narrow bands, while a crude approximation, still enables us to observe a possible cause of the observed singularities of invar alloys.

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ANOMALIES OF THE ELECTRONIC MAGNETIC SUSCEPTIBILITY OF A PLATE

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It is predicted that the diamagnetic susceptibility of a plate is subject to quasiperiodic temperature-independent oscillations due to electrons whose orbits are tangent to both plate boundaries. The calculation is performed in the one-electron approximation of band theory.

For a plate of thickness L, we investigated theoretically the dependence of the diamagnetic susceptibility χ on the magnetic field H parallel to the plate boundaries. The calculation was within the framework of the one-electron approximation of band theory in the quasiclassical approximation. We predict the existence of unique quasiperiodic oscillations of χ, which depend little on the temperature. The oscillations are due to internal (not Fermi) electrons. The oscillations should be observed not only in metals, but also in dielectrics with sufficiently broad bands.

Quantization of the electron energy in a magnetic field leads to a complicated dependence of the thermodynamic potential Ω of the electron gas on the magnetic field. Confining ourselves to the quasiclassical approximation (see below), we can say that each quantized orbit of the electron adds to Ω a contribution that contains a periodic function with argument $cS/e\hbar H$, where $S = S(\varepsilon, p_z, p_x)$ is the area inside the orbit traced by an electron having an energy ε and momentum projections p_x and p_z in momentum space (or part of the trajectory lying in the plate). The axes are chosen such that $H_z = H$ and $H_x = H_y = 0$; the y axis is perpendicular to the plate boundaries; the plate occupies the strip $0 < y < L$. Summation (integration) over all orbits results in contributions to the oscillating part of Ω (which we denote $\delta\Omega$) from orbits of electrons having an energy equal to the Fermi energy and an extremal area S, i.e., the electrons for which $\partial S/\partial p_z = 0$ (the de Haas - van Alphen effect, which is observed in metals and in degenerate semiconductors [1]). In the case of plates, however, $\delta\Omega$ receives contributions not only from these orbits, but also from orbits that are tangent to the two plate boundaries, and naturally satisfy the quantization condition

$$S(\epsilon, p_z) = (2\pi\hbar eH/c)(n + 5/6), \quad n = 1, 2, 3, \ldots \quad (1)$$