INFLUENCE OF COULOMB CORRELATIONS ON THE TYPE OF ORDERING AND ON THE EXISTENCE OF LOCALIZED MAGNETIC MOMENTS

By A. Stasch

Ferromagnetics Laboratory, Institute of Physics of the Polish Academy of Sciences, Poznań*

(Received December 1, 1969)

A problem of correlations of localized electrons affecting a character of mutual interactions of a localized pair of magnetic moments is considered in the Anderson's model. The method of a treatment of correlations of electrons in localized states, proposed by Hewson, was generalized for the case of an occurrence of interactions between localized moments. It is found that the possibility exists of both parallel and antiparallel orientations of localized moments in dilute alloys; with that, the parallel coupling is preferred.

1. Introduction

In recent times, a vast amount of work has been devoted to both experimental and theoretical research [1–17] on alloys consisting of non-magnetic metals with impurities of metals of the 3*d* group. As proved by the results, in well defined circumstances the impurity atoms preserve their spin magnetic moment related with the electrons in the strongly localized 3*d* states. This moment is termed the localized magnetic moment (L.M.M.). Its existence implies a number of interesting experimental effects, such as:

1. A change in character of the temperature dependence of the alloy's susceptibility to the Curie–Weiss one [1];

2. A temperature-dependence of the effective magnetic field at the impurity nucleus in the Mössbauer effect [2];

3. The appearence of a minimum of the electric resistivity at low temperatures (the Kondo effect) [3];

4. The occurrence of a localized spin density distribution in the neighbourhood of the impurity, as shown by neutron scattering experiments [4];

5. The possibility of a partial compensation of the impurity resistance by applying an external magnetic field [17].

All the experimental results can be predicted and explained on the basis of one of the existing theoretical models [5–9], among which Anderson's model is physically most valid

* Address: Zakład Ferromagnetyków, Instytut Fizyki PAN, Poznań, Fredry 10, Polska.

as regards the treatment of $3d$ group impurities. Within the framework of this model, the difference in character of the localized electron d states of the impurity as well as of the non-magnetic matrix bands in taken into account.

Our previous knowledge of the interactions and orderings of the L.M.M. is relatively scarce. In the present paper we shall use the Anderson model to discuss the effect of correlation of localized electron on the occurrence and interaction of pairs of localized moments. Preliminary results have been published recently [18].

2. *Hamiltonian of the system*

In Anderson's model [9], the assumption is made that the electrons of non-magnetic components of an alloy partially fill a single band; therefore, the Hamiltonian of the unperturbed matrix in the second quantization representation takes the following form:

$$H_b = \sum_{k\sigma} \varepsilon_{k\sigma} c^+_{k\sigma} c_{k\sigma} \tag{1}$$

ε_k is the kinetic energy of an electron in the $|k\sigma\rangle$ state, and $C^+_{k\sigma}$, $C_{k\sigma}$ are creation and annihilation operators of an electron in this state, respectively.

In our further considerations we shall use, as parameter of the theory, the position of the Fermi level only, and therefore we need not take into account the form of the band or recur to the many-band model. Instead, we make the standard assumption with respect to the occurrence of interaction with the band as well as mutual interaction between two impurity atoms. In addition, we assume that a free impurity atom is well described by a Hamiltonian of the form:

$$H = \sum_{i\sigma} E_0 c^+_{i\sigma} c_{i\sigma} + U n_{i\uparrow} n_{i\downarrow} \tag{2}$$

with E_0 denoting the kinetic energy of an electron in the d state of the i-th impurity, $C_{i\sigma}$, $C^+_{i\sigma}$ annihilation and creation operators of an electron in this state respectively, and $n_{i\sigma} = C^+_{i\sigma} C_{i\sigma}$ the occupation number operator;

$$U = e^2 \int |f_i(\vec{r})|^2 \frac{1}{|\vec{r} - \vec{r}'|} |f_i(\vec{r}')|^2 \, d\vec{r} d\vec{r}' \tag{3}$$

is the Coulomb interaction energy of the electrons in the states $|d\sigma\rangle$ and $|d-\sigma\rangle$. The value of U, evaluated from spectral data for free atoms, is very large and exceeds 10 eV [9]. When an impurity atom is introduced into the alloy, there appear interactions between electrons of the band and electrons of the impurity; due to the different symmetry and small overlap of the $3d$ wave functions with the states of the band. We take into account only couplings of the form:

$$\begin{aligned} H_{bi} &= \sum V_{ik} c^+_{i\sigma} c_{k\sigma} + \text{c.c.} \\ V_{ik} &= \int f_i(\vec{r}) v(\vec{r}) f_k(\vec{r}) d\vec{r} \end{aligned} \tag{4}$$

where $V(r)$ is the potential perturbing the band electrons and the impurity electrons, resulting by deformation of the periodical lattice potential and atomic shells of the impurity. The interaction (4) is due to the overlap of one d function with one band function. In the Coulomb

and exchange interactions there can however occur expressions relating with the overlapping of two localized functions with two band functions. Therefore such interactions can be predicted to be by one order of magnitude smaller than V_{ik}. From the experimental results, $V_{ik} \approx 1$ eV [9].

When a pair of impurity atoms is introduced into the alloy, there appears, moreover, a bilinear coupling between the impurity electrons:

$$H_{ij} = V_{ij} c_{i\sigma}^{+} c_{i\sigma} + \text{c.c.} \qquad i \neq j \tag{5}$$
$$V_{ij} = \int f_i^{*}(\vec{r}) v'(\vec{r}) f_j(\vec{r}) d\vec{r} \qquad i,j = 1,2$$

exchange as well as Coulomb interactions are neglected as for (4)). Considering the terms (1)–(5), we obtain the Hamiltonian of the system in the following form [16]:

$$H = \sum_{k\sigma} \varepsilon_k c_{k\sigma}^{+} c_{k\sigma} + \sum_{i\sigma} E_0 c_{i\sigma}^{+} c_{j\sigma} + U n_{1\uparrow} n_{1\downarrow} + U n_{2\uparrow} n_{2\downarrow} + \\ + \sum_{ki\sigma} V_{ik} c_{i\sigma}^{+} c_{k\sigma} + V_{12} c_{1\sigma}^{+} c_{2\sigma} + \text{c.c.} \tag{6}$$

3. *Criterion for the occurrence and ordering of mutually interacting localized magnetic moments*

In our further considerations we intend to use the Green function method [13] and, particularly, shall recur to relations between Fourier transforms of Green's functions and values of the correlation function $\langle B(t')\, A(t)\rangle$ of two appropriate operators $A(t)$, $B(t')$ acting on variables of the system. On the base of the Green function theory, one obtains that

$$\langle B(t')\, A(t)\rangle = -i \int_{-\infty}^{\infty} \frac{\langle\langle A(t); B(t')\rangle\rangle_{\omega+i\varepsilon} - \langle\langle A(t); B(t')\rangle\rangle_{\omega+i\varepsilon}}{e^{\beta(\omega-\varepsilon_F)}+1} e^{i\omega(t-t')}\, d\omega \tag{7}$$

where $\beta = 1/\mathrm{kT}$

and

$$\langle\langle A(t); B(t')\rangle\rangle_{\omega} = \frac{1}{2\pi} \int_{-\infty}^{\infty} \langle\langle A(t); B(t')\rangle\rangle\, e^{-i\omega(t-t')} d(t-t') \tag{7a}$$

is the Fourier transform of the double-time Green function

$$\langle\langle A(t); B(t')\rangle\rangle = -i\Theta(t-t')\langle [A(t), B(t')]\rangle \tag{7b}$$
$$\Theta(t-t') = 1 \quad \text{for} \quad t > t'$$
$$0 \quad \text{for} \quad t < t'$$

taking

$$c_{d\sigma}^{+} = B \qquad c_{d\varrho} = A \qquad t' = t + 0^{\pm} \tag{8}$$

and carrying out the calculations for the ground state of the system ($\beta \to \infty$), we obtain for the average occupation numbers of the localized state of the i-th impurity as well as for the energy of the impurity electron system the following expressions, respectively,

$$\bar{n}_{i\sigma} = \int_{-\infty}^{\varepsilon_F} \varrho_{i\sigma}(\omega) d\omega \tag{9}$$

$$E = \sum_{i\sigma} \int^{\varepsilon_F} \omega \varrho_{i\sigma}(\omega) d\omega \tag{10}$$

where

$$\varrho_{i\sigma}(\omega) = -i \lim_{\varepsilon \to 0} [G^{\sigma}_{ii}(\omega + i\varepsilon) - G^{\sigma}_{ii}(\omega - i\varepsilon)] \tag{11}$$

$$G^{\sigma}_{ii}(\omega) = \langle\langle c_{i\sigma}; c^{+}_{i\sigma} \rangle\rangle_{\omega}. \tag{11a}$$

Using (10) we can calculate the difference in energy between the antiparallel and parallel ordered L.M.M., given by the relation:

$$\Delta E = E_{\uparrow\downarrow} - E_{\uparrow\uparrow} = \sum_{i\sigma} \int^{\varepsilon_F} \omega (\varrho^{ap}_{i\sigma} - \varrho^{p}_{i\sigma}) d\omega \tag{12}$$

where $\varrho^{p}_{i\sigma}$ and $\varrho^{ap}_{i\sigma}$ denote the spectral densities of the states $|i\sigma\rangle$ for the parallel and antiparallel L.M.M., respectively.

In order to discuss the properties of the system described by the Hamiltonian (6) we thus have to find the function $G^{\sigma}_{ii}(\omega)$. This function can be obtained from the following set of equations of motion:

$$(\omega - E_0) \langle\langle c_{i\sigma}; c^{+}_{i\sigma} \rangle\rangle_{\omega} = \frac{1}{2\pi} + U \langle\langle c_{i\sigma} n_{i-\sigma}; c^{+}_{i\sigma} \rangle\rangle + \sum_{k} V_{ik} \langle\langle c_{k\sigma}; c^{+}_{i\sigma} \rangle\rangle_{\omega} + V_{12} \langle\langle c_{j\sigma}; c^{+}_{i\sigma} \rangle\rangle_{\omega} \tag{13a}$$

$$(\omega - \varepsilon_k) \langle\langle c_{k\sigma}; c^{+}_{i\sigma} \rangle\rangle_{\omega} = V_{ki} \langle\langle c_{i\sigma}; c^{+}_{i\sigma} \rangle\rangle_{\omega} + V_{kj} \langle\langle c_{j\sigma}; c^{+}_{i\sigma} \rangle\rangle_{\omega} \qquad i \neq j \tag{13b}$$

$$(\omega - E_0) \langle\langle c_{j\sigma}; c^{+}_{i\sigma} \rangle\rangle_{\omega} = U \langle\langle n_{j-\sigma} c_{j\sigma}; c^{+}_{i\sigma} \rangle\rangle_{\omega} + \sum_{k} V_{jk} \langle\langle c_{k\sigma}; c^{+}_{i\sigma} \rangle\rangle + V_{ji} \langle\langle c_{i\sigma}; c^{+}_{i\sigma} \rangle\rangle_{\omega} \tag{13c}$$

$$\begin{aligned}(\omega - E_0 - U) \langle\langle c_{i\sigma} n_{i-\sigma}; c^{+}_{i\sigma} \rangle\rangle_{\omega} = {} & \frac{\bar{n}_{i-\sigma}}{2\pi} + \sum_{k} V_{ik} \langle\langle c_{k\sigma} n_{i-\sigma}; c^{+}_{i\sigma} \rangle\rangle_{\omega} + \\ & + \sum_{k} V_{ik} \langle\langle c^{+}_{k-\sigma} c_{i\sigma} c_{i-\sigma}; c^{+}_{i\sigma} \rangle\rangle_{\omega} + \sum_{k} V_{ik} \langle\langle c_{k-\sigma} c_{i\sigma} c^{+}_{i-\sigma}; c^{+}_{i\sigma} \rangle\rangle_{\omega} + \\ & + V_{ij} \langle\langle c_{j\sigma} n_{i-\sigma}; c^{+}_{i\sigma} \rangle\rangle_{\omega} + V_{ij} \langle\langle c^{+}_{j-\sigma} c_{i\sigma} c_{i-\sigma}; c^{+}_{i\sigma} \rangle\rangle_{\omega} + V_{ij} \langle\langle c_{j-\sigma} c_{i\sigma} c^{+}_{i-\sigma}; c^{+}_{i\sigma} \rangle\rangle_{\omega}.\end{aligned} \tag{13d}$$

Before proceeding to discuss the set of equations (13), we shall make some simplifying assumptions. Namely, we shall neglect functions of the type $\langle\langle c^{+}_{k-\sigma} c_{i\sigma} c_{i-\sigma}; c^{+}_{i\sigma} \rangle\rangle$, $\langle\langle c^{+}_{j-\sigma} c_{i\sigma} c_{i-\sigma}; c^{+}_{i\sigma} \rangle\rangle$, $\langle\langle c_{k-\sigma} c_{i\sigma} c^{+}_{i-\sigma}; c^{+}_{i\sigma} \rangle\rangle$ and $\langle\langle c_{j-\sigma} c_{i\sigma} c^{+}_{i-\sigma}; c^{+}_{i\sigma} \rangle\rangle$ for $i \neq j$.
The first and second of these provide non-zero contributions only for transitions of the system to unperturbed states, in which the levels $|i\sigma\rangle$ and $|i-\sigma\rangle$ are simultaneously occupied, increasing the energy of the system by the value U. Transitions of this type under the influence of the perturbation $V_{ik} \ll U$ have, however, a very small probability. The third and the fourth function does not affect the occurrence of non-interacting L.M.M. [10]. We apply the Hartree-Fock approximation for the Green functions the form $\langle\langle c_{k\sigma} n_{i-\sigma}; c^{+}_{i\sigma} \rangle\rangle_{\omega}$ $\langle\langle c_{j\sigma} n_{i-\sigma}; c^{+}_{i\sigma} \rangle\rangle_{\omega}$ and $\langle\langle c_{j\sigma} n_{j-\sigma}; c^{+}_{i\sigma} \rangle\rangle_{\omega}$ when $i \neq j$ using the following relations

$$\langle\langle c_{k\sigma} n_{i-\sigma}; c_{i\sigma}^{+}\rangle\rangle_{\omega} \approx \bar{n}_{i-\sigma}\langle\langle c_{k\sigma}; c_{i\sigma}^{+}\rangle\rangle_{\omega}$$

$$\langle\langle c_{j\sigma} n_{i-\sigma}; c_{i\sigma}^{+}\rangle\rangle_{\omega} \approx \bar{n}_{i-\sigma}\langle\langle c_{j\sigma}; c_{i\sigma}^{+}\rangle\rangle_{\omega}$$

$$\langle\langle c_{j\sigma} n_{j-\sigma}; c_{i\sigma}^{+}\rangle\rangle_{\omega} \approx \bar{n}_{j-\sigma}\langle\langle c_{j\sigma}; c_{i\sigma}^{+}\rangle\rangle_{\omega} \tag{14}$$

where $\bar{n}_{i-\sigma}$ stands for the average occupations number of electrons in the localized states. The function $\langle\langle c_{i\sigma} n_{i-\sigma}; c_{i\sigma}^{+}\rangle\rangle$ is obtained from the equations of motion. After performing the simplifications specified by (14) the equations (13c), (13d) take the following form

$$(\omega - E_0 - U)\,\langle\langle c_{j\sigma}; c_{i\sigma}^{+}\rangle\rangle_{\omega} = \sum_{v} V_{jk}\langle\langle c_{k\sigma}; c_{i\sigma}^{+}\rangle\rangle_{\omega} + V_{ji}\langle\langle c_{i\sigma}; c_{i\sigma}^{+}\rangle\rangle \tag{15}$$

$$(\omega - E_0 - U)\langle\langle c_{i\sigma} n_{i-\sigma}; c_{i\sigma}^{+}\rangle\rangle_{\omega} = \frac{\bar{n}_{i-\sigma}}{2\pi} + \bar{n}_{i-\sigma}\sum_{k} V_{ik}\langle\langle c_{k\sigma}; c_{i\sigma}^{+}\rangle\rangle_{\omega} + \bar{n}_{i-\sigma} V_{ij}\langle\langle c_{j\sigma}; c_{i\sigma}^{+}\rangle\rangle_{\omega}. \tag{16}$$

The preceding method of dealing with the double-particle Green functions is essentially superior to the Hartree-Fock method used in the papers of Anderson and Alexander [16] as well as Moriya [14] in that leads to exact eigenstates of the unperturbed Hamiltonian in the limit $V_{12}, V_{ik} \to 0$. The use of the H–F approximation for the correlation function $\langle c_{i\sigma} n_{i-\sigma} c_{i\sigma}^{+}\rangle$ strongly raises the tendency towards the occurrence of L. M. M. by overrating the Coulomb interaction energy of electrons simultaneously occupying the two spin states $|i\sigma\rangle$ and $|i-\sigma\rangle$ of the impurity (see also: [10, 11, 15]). The splitting of the form $\langle\langle c_{i\sigma} n_{i-\sigma}; c_{i\sigma}^{+}\rangle\rangle = \bar{n}_{i-\sigma}\langle\langle c_{i\sigma}; c_{i\sigma}^{+}\rangle\rangle$ used in the H—F method means that we treat an electron in the $|i\sigma\rangle$ state as being in an average Coulomb field of an electron in the $|i-\sigma\rangle$ state; this amounts to neglecting the fact that the motion of impurity electrons is correlated.

In our further discussion, using the set of Eqs (16) as well as (9) – (12) we shall draw certain important qualitative conclusions. For simplicity, we shall confine our considerations to terms of the order $1/U$ at most; moreover we omit the indirect coupling of electrons in the localized states *via* the conduction electrons (see also [16]).

Finally, we obtain for $G_{ii}^{\sigma}(\omega)$ and $\varrho_{i\sigma}(\omega)$ the following expressions

$$G_{ii}^{\sigma}(\omega + i\varepsilon) = \frac{1}{2\pi} \times \frac{(1-\bar{n}_{i-\sigma})}{\left[\omega - E_0 - \left(\lambda - \dfrac{V_{12}^2}{U\bar{n}_{j-\sigma}}\right)\right] + i\Delta(1-\bar{n}_{i-\sigma})} \tag{17}$$

$$\varrho_{i\sigma}(\omega) = \frac{1}{\pi} \frac{\Delta(1-\bar{n}_{i-\sigma})^2}{\left[\omega - E_0 - \left(\lambda - \dfrac{V_{12}^2}{U\bar{n}_{j-\sigma}}\right)(1-\bar{n}_{i-\sigma})\right]^2 + \Delta^2(1-\bar{n}_{i-\sigma})^2} \tag{18}$$

where

$$\lambda = P\sum_{k} \frac{|V_{ik}|^2}{\omega - \varepsilon_k} \tag{19}$$

$$\Delta = \lim_{\varepsilon \to 0+} \mathrm{Im} \sum_{k} \frac{|V_{ik}|^2}{\omega - \varepsilon_k + i\varepsilon} = -\pi\, \bar{V}_{ik}^2 \varrho_{k\sigma}(\omega). \tag{20}$$

Making use of Anderson's assumption [9] according to which λ and Δ are slow-varying functions of the energy, or $\varrho_{k\sigma}(\omega) = \text{const}$ in the vicinity of the Fermi level we obtain

$$\bar{n}_{i\sigma} = \frac{1-\bar{n}_{i-\sigma}}{\pi}\left[\tan^{-1}\frac{E_F-E_0-(1-\bar{n}_{i-\sigma})\left(\lambda-\frac{\bar{V}_{12}^2}{U\bar{n}_{j-\sigma}}\right)}{\Delta(1-\bar{n}_{i-\sigma})}+\frac{\pi}{2}\right]. \tag{21}$$

Using the relations (21) and (9), we can now find systems of self-consistent equations for obtaining the occupation numbers of the localized states for parallel ordering *i. e.* for $\bar{n}_{1\sigma} = \bar{n}_{2\sigma} = n_\sigma$ as well as for antiparallel ordering *i. e.* for $\bar{n}_{1\sigma} = \bar{n}_{2-\sigma} = m_\sigma$,

$$n_\sigma = \frac{1-n_{-\sigma}}{\pi}\left[\tan^{-1}\frac{E_F-E_0-(1-n_{-\sigma})\left(\lambda-\frac{\bar{V}_{12}^2}{Un_{-\sigma}}\right)}{\Delta(1-n_{-\sigma})}+\frac{\pi}{2}\right] \tag{22}$$

$$m_0 = \frac{1-n_{-\sigma}}{\pi}\left[\tan^{-1}\frac{E_F-E_0-(1-m_{-\sigma})\left(\lambda-\frac{\bar{V}_{12}^2}{Um_\sigma}\right)}{\Delta(1-m_{-\sigma})}+\frac{\pi}{2}\right]. \tag{23}$$

Using the relations (22) and (23) we shall now determine the criterion for the occurrence of L. M. M. for a definite ordering and then, using (12), we shall discuss the problem of stability of the ordering in the region in which L. M. M. occurs for both parallel and antiparallel coupling. Thus, the curve bounding that range of values of the parameters of the model in which L. M. M. occurs can be obtained from the following conditions:

1. On the curve itself L. M. M. defining as $n_\uparrow - n_\downarrow$ or $m_\uparrow - m_\downarrow$ is still equal to zero *i. e.*

$$n_\uparrow = n_\downarrow = m_\downarrow = m_\uparrow = n_c. \tag{24}$$

2. In the region of occurrence of L. M. M., solutions of the form $n_\uparrow \neq n_\downarrow$ or $m_\uparrow \neq m_\downarrow$ must appear *i. e.*

$$\frac{\partial n^\uparrow}{\partial n_\downarrow} \leqslant -1 \quad \text{or} \quad \frac{\partial m^\uparrow}{\partial m_\downarrow} \leqslant -1 \tag{25}$$

(equality takes place on the bounding curve itself [16]). Defining dimensionless parameters of the theory as follows:

$$x = \frac{E_0-E_F}{\Delta} \qquad y = \frac{-\lambda}{\Delta} \qquad z = \frac{\bar{V}_{12}^2}{U\Delta} \tag{26}$$

we obtain from (24) and (24) parametric equations for x, y and z values on the bounding curve for parallel and antiparallel L. M. M. coupling, respectively,

$$x_p = (1-2n_c)\pi\left\{1+\left[\tan\frac{(3n_c-1)\pi}{2(1-n_c)}\right]^2\right\} - \left(\frac{1-n_c}{n_c}\right)^2 \tag{27a}$$

$$y_p = \tan\frac{(3n_c-1)\pi}{(1-n_c)2} + \frac{x_p}{1-n_c} - \frac{z_p}{n_c} \tag{27b}$$

$$x_{ap} = (1-2n_c)\pi \left\{1 + \left[\tan\frac{(3n_c-1)\pi}{(1-n_c)2}\right]^2 + \left(\frac{1-n_c}{n_c}\right)^2\right. \tag{28a}$$

$$y_{ap} = \tan\frac{(3n_c-1)\pi}{(1-n_c)2} + \frac{x_{ap}}{1-n_c} - \frac{z_{ap}}{n_c}. \tag{28b}$$

The regions of occurrence of localized magnetic moments as well as the bounding curves for both ordering and for interaction parameters $z = 0.05; 0.10; 0.15$ are given in Figs 1–3. These diagrams permit certain interesting conclusions concerning the influence of the bilinear interaction V_{12} on the region of occurrence and ordering of L. M. M. As seen, the parallel ordering can generally occur in narrower region of values of the parameters x, y as well as for values of $x = \dfrac{E_0 - E_F}{\Delta}$ closer to zero. In other words, the parallel orientation of L. M. M. occurs when an unperturbed level of an impurity atom E_0 lies nearer the Fermi level. The most interesting result seems to consist in an increasing splitting of regions of occurrence of L. M. M. for parallel and antiparallel orderings when the interaction V_{12} increase. Such splitting allows us to go over from alloys with no L. M. M. *via* alloys with parallel-ordered moments to antiparallel systems by gradual emptying of the conduction

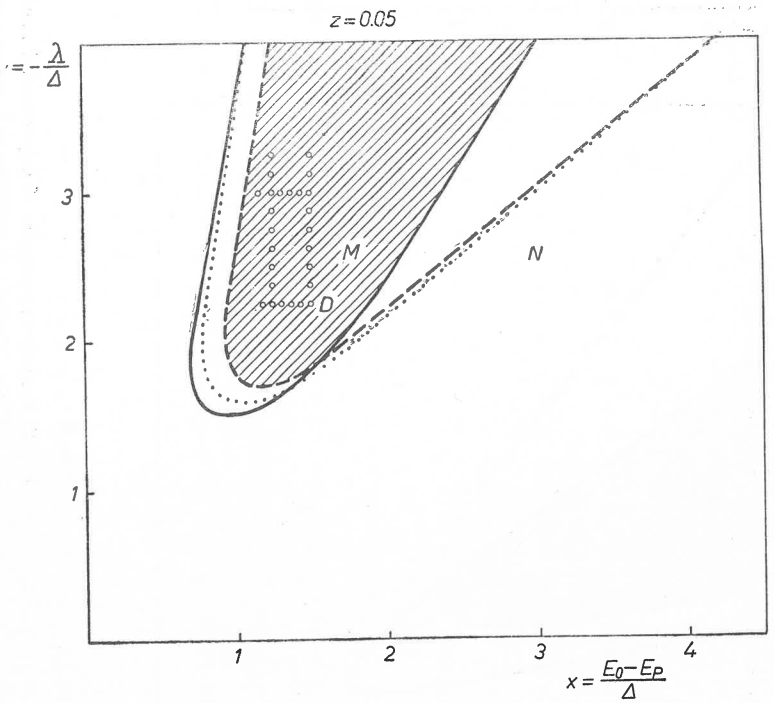

Fig. 1. Critical boundaries for the existence of magnetic solutions for $z = 0.05$. The dotted curve corresponds to non interacting impurity ($z = 0$). In the region above full line there appear localized magnetic moments coupled parallelly, similarly the broken line determines the domain of existence for antiparallel configuration of localized magnetic moments

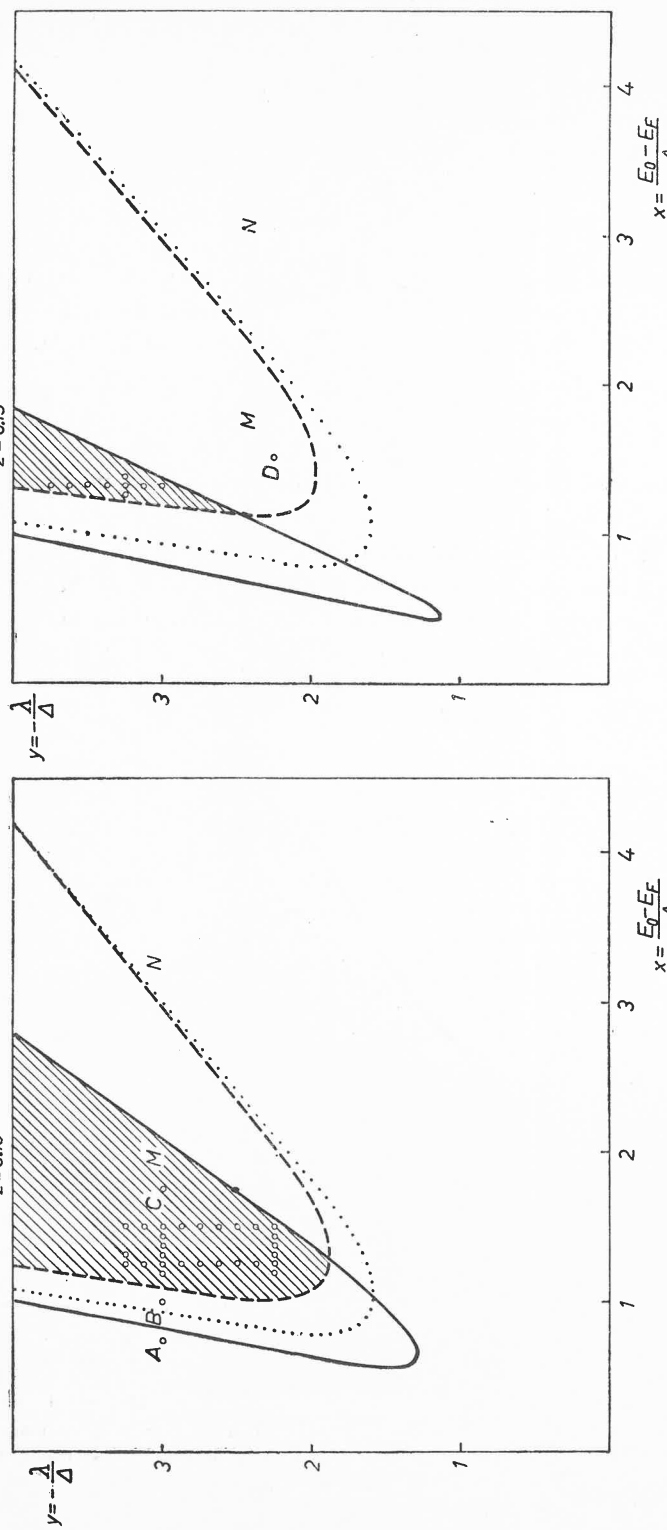

Fig. 2

Fig. 3

Fig. 2. Regions of existence of magnetic and nonmagnetic soluions for $z = 0.10$

Fig. 3. Regions of magnetic and nonmagnetic solutions for $z = 0.15$

band. Increasing or decreasing of an occupation of the conduction band of the non-magnetic matrix can be attained by introducing to the matrix metals with larger or smaller number of valence electrons, respectively. As shown in Figs 1–3, a change in ordering or disappearence of L. M. M. can be also obtained by varying the interaction parameter z, which depends on the concentration of magnetic impurities. The graphs of the occupation numbers (Figs 4–6) in the points A (0.75, 3.0), B (1.25, 3.0), C (1.75, 3.0) show how the localized moment varies with decreasing filling of the band for parallel and antiparallel ordering. As

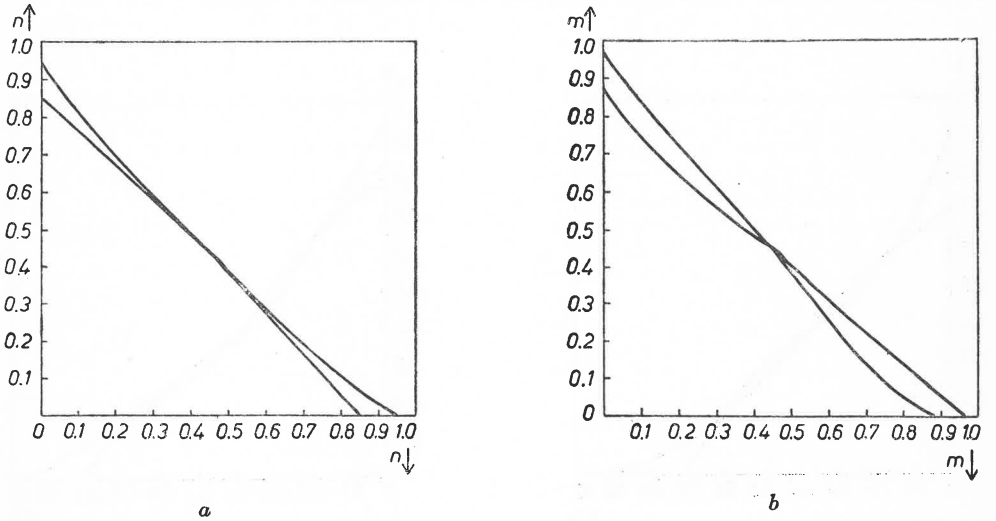

Fig. 4*a*. Plot of $n_\uparrow$ ($n_\downarrow$) and $n_\downarrow$ ($n_\uparrow$) for values of $x = 0.75$, $y = 3.0$, $z = 0.1$. The point A in Fig. 2. The curves are computed from Eq. (22). *b*. Plot $m_\uparrow$ *versus* $m_\downarrow$ and $m_\downarrow$ *versus* $m_\uparrow$ for x, y, z parameters as in Fig. 4*a*

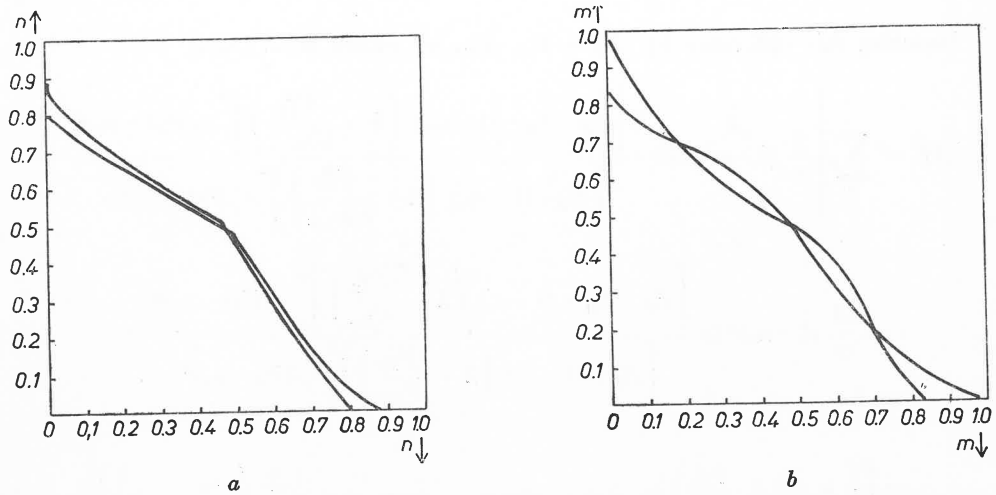

Fig. 5*a*. The dependence of $n_\uparrow$ on $n_\downarrow$ and $n_\downarrow$ on $n_\uparrow$ for $x = 1.0$, $y = 3.0$, $z = 0.1$. The point B in Fig. 2. *b*. Plot of $m_\uparrow$ ($m_\downarrow$) and $m_\downarrow$ ($m_\uparrow$). Parameters x, y, z are the same as for Fig. 5*a*

seen, in the point A, L. M. M. disappears for both orderings (*i. e.* only the non-magnetic solution $n_\uparrow = n_\downarrow$ occurs); in the point B, L. M. M. appears for the ferromagnetic case (we have $n_\uparrow = 0,71$, $n_\downarrow = 0.18$ *i. e.* $M = M_B\,(n_\uparrow - n_\downarrow) = 0.53\,M_B$) and, in the point C, the magnetic solution $n_\uparrow \neq n_\downarrow$ occurs for both orderings. The occurrence criterion thus enables us to draw a number of qualitative conclusions as regards ordering in the region of parameters where the ranges of occurrence of L. M. M. for both orderings do not overlap; on the other hand in the range of overlapping (the shaded area in Figs 1–3), one has to calculate the difference in energy for parallel and antiparallel coupling.

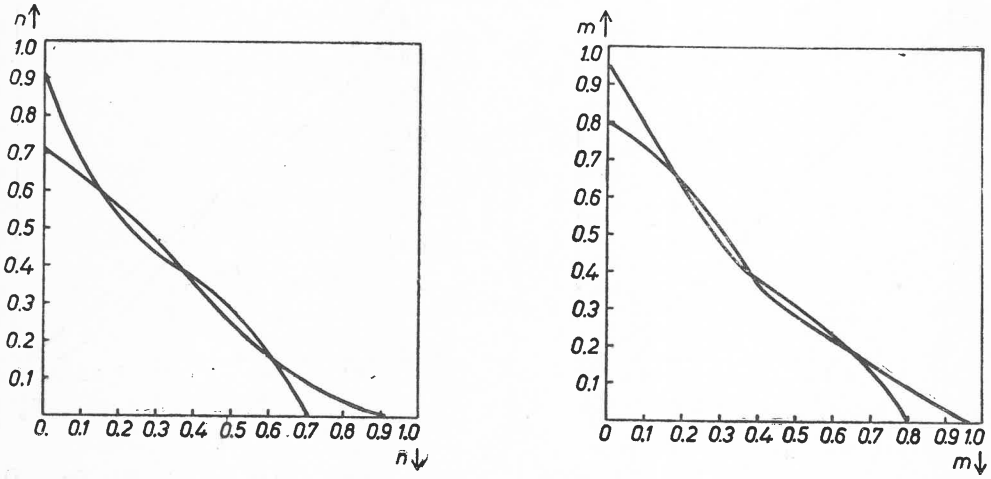

Fig. 6*a*. Calculated curves for $n_\uparrow$ *versus* $n_\downarrow$ and $m_\downarrow$ *versus* $n_\uparrow$ for values of $x = 1.75$, $y = 3.0$, $z = 0.1$. The point C in Fig. 2. *b*. Plot $m_\uparrow$ $(m_\downarrow)$ and $m_\downarrow$ $(m_\uparrow)$. The x, y, z parameters are the same as in Fig. 6*a*

Denoting this difference by $\Delta E = E_{\uparrow\downarrow} - E_{\uparrow\uparrow}$, we obtain from (12):

$$\Delta E = \sum_\sigma \left\{ \frac{\Delta}{\pi}(1-m_\sigma)^2 \ln \frac{\left[E_F - E_0 - (1-m_\sigma)\left(\lambda - \frac{V_{12}^2}{Um_{-\sigma}}\right)\right]^2 + \Delta^2(1-m_\sigma)^2}{\left[E_0 + (1-m_\sigma)\left(\lambda - \frac{V_{12}^2}{Um_{-\sigma}}\right)\right]^2 + \Delta^2(1-m_\sigma)^2} + \right.$$

$$+ \frac{\Delta}{\pi}(1-n_\sigma)^2 \ln \frac{\left[E_F - E_0 - (1-n_\sigma)\left(\lambda - \frac{V_{12}^2}{Un_\sigma}\right)\right]^2 + \Delta^2(1-n_\sigma)^2}{\left[E_0 + (1-n_\sigma)\left(\lambda - \frac{V_{12}^2}{Un_\sigma}\right)\right]^2 + \Delta^2(1-n_\sigma)^2} -$$

$$\left. - 2\left[\left(E_0 + \lambda + \frac{V_{12}^2}{U}\right)(n_\sigma - m_\sigma) + \lambda(n_\sigma n_{-\sigma} - m_\sigma m_{-\sigma}) + \frac{V_{12}^2}{U}\left(\frac{n_\sigma}{n_{-\sigma}} - 1\right)\right]\right\} \qquad (29)$$

where n_σ and m_σ are the solutions of the sets of Eqs (22) and (23), respectively. In the strongly magnetic case $n_\uparrow - n_\downarrow \approx m_\uparrow - m_\downarrow \approx 1$

$$\Delta E \approx \frac{2V_{12}^2}{U}\left(\frac{n_\uparrow}{n_\downarrow} + \frac{n_\downarrow}{n_\uparrow}\right) \approx \frac{2V_{12}^2}{U}\,\frac{n_\uparrow}{n_\downarrow} > 0 \tag{30}$$

pointing to stability of the ferromagnetic ordering. The same analytic result is obtained in the magnetic case and if $\Delta \to 0$. Here in the magnetic solutions $n_\uparrow - n_\downarrow \approx m_\uparrow - m_\downarrow \approx 1$. A more detailed discussion of the stability problem of L. M. M. orderings by numerical methods is shown in Figs 7–12. In our numerical calculations we have taken $E_0 = 2\,\mathrm{eV}$, $\Delta = 0.5$ eV, and the values of variables x, y for which ΔE has been calculated are represented by circles in the diagrams 1–3. By our analysis of these diagrams, the tendency to parallel L. M. M. ordering is clearly apparent. We conclude that energy considerations favour ferromagnetism in the range in which L. M. M. can occur.

Accordingly, in the majority of cases, parallel L. M. M. ordering is expected to occur in alloys. On the other hand, antiparallel ordering occurs only for large values of z *i. e.* for large concentrations of magnetic impurities (Fig. 3). Moreover, as seen from Figs 1–3, for a certain region of values of the Fermi energy we can induce the change from parallel to antiparallel L. M. M. ordering by increasing z (by varying the concentrations of magnetic

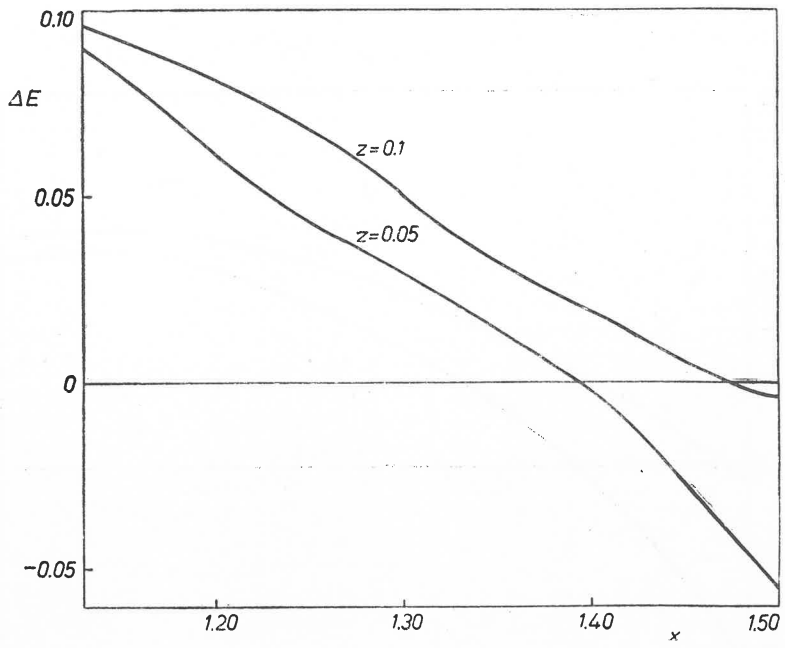

Fig. 7. Relative stability of the parallel and antiparallel configurations of localized magnetic moments. The curves of the energy difference $\Delta E = E_{\uparrow\downarrow} - E_{\uparrow\uparrow}$ *versus* x were calculated for $y = 2.25$, $z = 0.05$ and 0.1 respectively

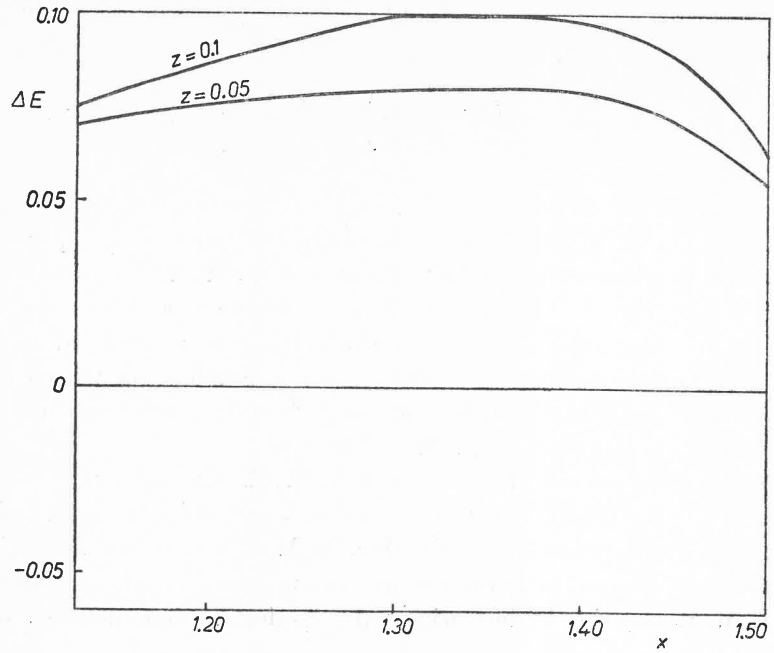

Fig. 8. Plot ΔE *vs* x for $y = 3.00$. Other parameters are the same as for Fig. 7

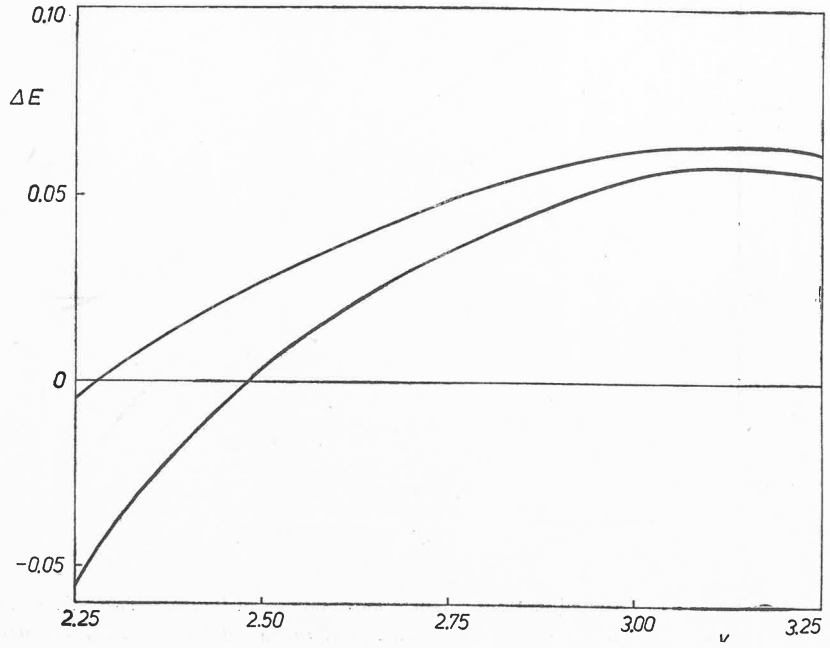

Fig. 9. The dependence of the energy difference ΔE on the parameter x for $y = 3.25$, $z = 0.15$

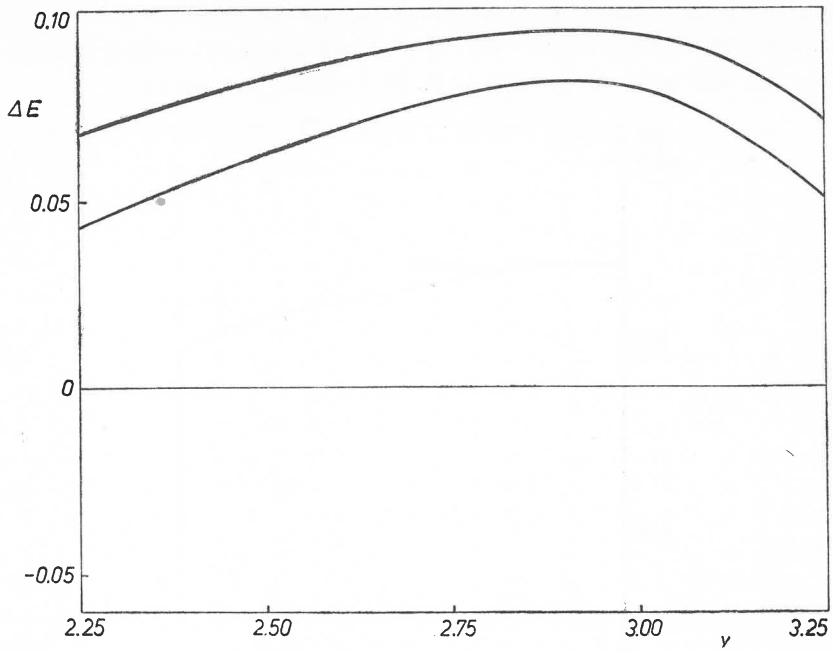

Fig. 10. The E as function of $y = -\frac{\lambda}{\Delta}$ for $x = 1.25$, $z = 0.05$ and 0.10 respectively

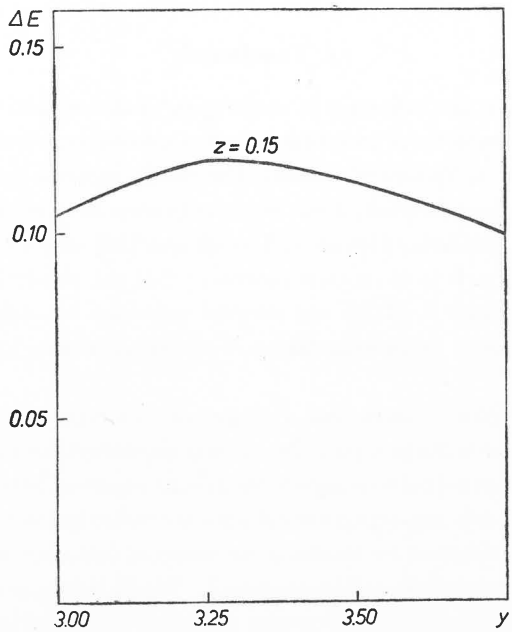

Fig. 11. The dependence of ΔE on the parameter y for $x = 1.50$ and remaining parameters as in Fig.1

impurities). This is immediately apparent on considering the properties of the system in Figs 1–3 in the point $D(1.3, 2.25)$. For $z = 0.1$, parallel ordering shows stability (see also: Fig. 7), whereas for $z = 0.15$ only antiparallel L. M. M. coupling can appear.

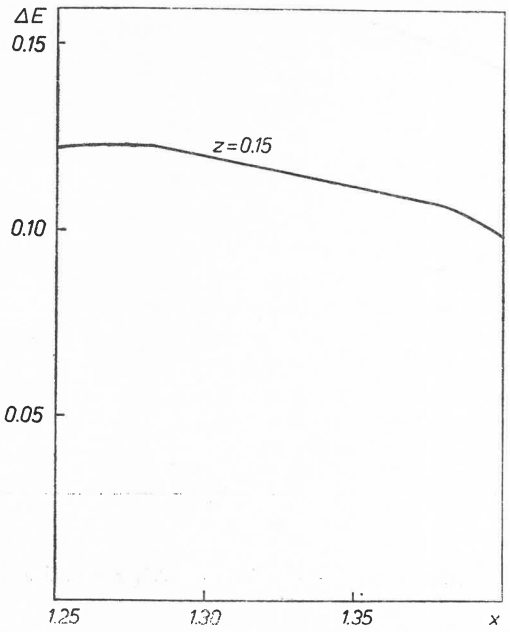

Fig. 12. Plot ΔE *versus* y for values $x = 1.30$, $z = 0.15$

4. *Conclusions*

In the present paper, the influence of correlation of the motion of electrons localized at impurity atoms on the character of coupling as well as on the occurrence of L. M. M. has been investigated on the basis of Anderson's model. The results indicate that the parallel orderings is favoured and thus differ essentially from the conclusions derived in the H–F approximation by Anderson and Alexander [16] as well as Moriya [14] where both orderings have the same domein of existence. It is of interest moreover that the possibility exists of transitions from system with quenched L. M. M. *via* parallel orderings to antiparallel systems, which are expected to appear with decreasing filling of the band of non-magnetic matrix of alloy (lowering of E_F).

Moreover the calculations show that changes of this type can also be obtained at an established filling of the conduction band by varying the concentrations of magnetic impurities. Finally, it would seem useful to compare the results obtained here with the experimental data. Unfortunately, the existing experimental data are restricted to very low concentrations, at which the effects of interaction of localized moments at impurity atoms are not important.

Our conclusion that parallel configuration of L. M. M. is energetically favoured leading to ferromagnetism at low temperatures seems to find a confirmation in the fact that this ordering is the only one occurring in alloys PdFe, PtFe.

The interpretation of coupling in such systems is, however, made more difficult by the occurrence of the so-called "giant moment", that is of L. M. M. of magnitude up to $12\mu_B$ per 1 atom of the impurity which is related to the polarization of Pd atoms by the impurity.

The authors thanks are due to Dr J. Morkowski for calling this problem to his attention and for many valuable discussions.

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