

QUANTITATIVE CRITERION FOR FERROMAGNETISM

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The difference between the energies of the nonmagnetic and ferromagnetic states of a metal is calculated in the Hartree-Fock approximation by using the one-electron functions obtained by using the spherical cellular method of Wigner and Seitz. For V, Fe, and Ni the ferromagnetic state was found to be favored. For Nb, Ru, and Pd both energies are essentially the same.

IT is well-known that the fundamental difficulty in obtaining a quantitative criterion for ferromagnetism in band theory is associated with the need to take correlation effects into consideration, i.e., a result beyond the scope of the Hartree-Fock (HF) approximation. However, the results in the HF approximation apparently remain valid if the metal turns out to be nonmagnetic<sup>[1]</sup> in this approximation. The question remains open if the metal turns out to be magnetic in the HF approximation. In the present article three elements of the iron group, V, Fe, and Ni, are considered in the HF approximation, and also the triplet Nb, Ru, and Pd standing under them.

The calculations were carried out on the basis of the energy bands and eigenfunctions obtained by using the self-consistent Hartree method in the spherical Wigner-Seitz approximation.<sup>[2]</sup> The elements V, Fe, and Ni satisfy the condition necessary for ferromagnetism. For metals of the Pd group the energies of the ferromagnetic and nonmagnetic states are essentially the same. In order to exclude V or Nb it is apparently necessary to go beyond the framework of the Hartree-Fock approximation. The energy difference between the magnetic and nonmagnetic states for Fe and Ni exceeds the Curie temperature by more than an order of magnitude, and obviously does not have any relation to it since the state of the metals above the Curie temperature is not nonmagnetic but paramagnetic.

1. GENERAL EXPRESSION FOR THE ENERGY OF A CRYSTAL

We give here a general expression for the energy of the electronic system of a crystal associated with different values of the average magnetic moment  $\mu$  belonging to one of its atoms.

The state with a given value of  $\mu$  is stable if it is energetically more favorable compared to the other states. Thus, the problem reduces to a computation of the curve

$$\Delta E(\mu) \equiv E(\mu) - E(0), \tag{1.1}$$

where  $E(\mu)$  and  $E(0)$  denote the crystal's energy in the magnetic and nonmagnetic states, respectively.

For the nonrelativistic case, in the HF approximation the energy of the electronic system in atomic units of energy (1 atomic unit of energy =  $me^4/\hbar^2 = 27.2$  eV) is given by<sup>[3]</sup>

$$E_{HF} = \sum^+ \int \Psi_i^* \left( -\frac{\Delta}{2} + U \right) \Psi_i dr + \sum^- \int \Psi_i^* \left( -\frac{\Delta}{2} + U \right) \Psi_i dr$$

$$+ \frac{1}{2} \iint \frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} d\mathbf{r} d\mathbf{r}' - \frac{1}{2} \iint \frac{|\rho_+(\mathbf{r}|\mathbf{r}')|^2 + |\rho_-(\mathbf{r}|\mathbf{r}')|^2}{|\mathbf{r}-\mathbf{r}'|} d\mathbf{r} d\mathbf{r}'. \tag{1.2}$$

Here the  $\psi_i(\mathbf{r})$  are the spatial parts of the one-electron functions,  $\sum^\pm$  denote sums over the electron states with spin + or -, respectively,  $U(\mathbf{r})$  denotes the potential of the nucleus, and

$$\rho_\pm(\mathbf{r}|\mathbf{r}') \equiv \sum_i^\pm \Psi_i^*(\mathbf{r}') \Psi_i(\mathbf{r}), \quad \rho(\mathbf{r}) = \rho_+(\mathbf{r}|\mathbf{r}) + \rho_-(\mathbf{r}|\mathbf{r}).$$

Let us represent (1.2) in symbolic form ( $E_{ex}$  denotes the last term in (1.2)):

$$E_{HF} = E_H(\Psi_{HF}) + E_{ex}(\Psi_{HF}).$$

Now it is easy to estimate the error introduced into (1.2) by replacing the spatial parts of the Hartree-Fock one-electron functions  $\psi_{HF}$  by the Hartree functions  $\psi_H$ . Since the functions  $\psi_{HF}$  minimize  $E_{HF}$ , and the functions  $\psi_H$  minimize  $E_H$ , then

$$E_H(\Psi_H) - E_H(\Psi_{HF}) < 0, \\ E_{HF}(\Psi_H) - E_{HF}(\Psi_{HF}) = E_H(\Psi_H) - E_H(\Psi_{HF}) + E_{ex}(\Psi_H) - E_{ex}(\Psi_{HF}) > 0.$$

Therefore

$$0 < E_{HF}(\Psi_H) - E_{HF}(\Psi_{HF}) < E_{ex}(\Psi_H) - E_{ex}(\Psi_{HF}),$$

i.e., the error in  $E_{HF}$  is smaller than the error introduced into  $E_{ex}$  in this connection. Calculations by V. G. Podval'nyi (private communication) show that  $\psi_{HF}$  does not differ markedly from  $\psi_H$ , so that the error in  $E_{ex}$  is small in comparison with  $E_{ex}$ . In what follows we shall use  $\psi_H$ .

The energy  $E_H(\mu)$  changes relatively little upon a change of  $\mu$ , but since  $E_H \gg E_{ex}$  formula (1.1) leads to the evaluation of a small difference between large quantities.<sup>1)</sup> In order to by-pass this difficulty we apply Koopmans' theorem (see, for example,<sup>[4]</sup>), having modified it in an appropriate way: the change of  $E_H(\mu)$  associated with the transfer of a portion  $dN$  of the electrons from the level  $E_F^-(\mu)$  to the level  $E_F^+(\mu)$  is equal to  $dN(E_F^+ - E_F^-)$ .

Then the difference between the Hartree energies is given by

$$E_H(\mu) - E_H(0) = \int_0^\mu [E_{F_n^+}(\mu) - E_{F_n^-}(\mu)] N d\mu. \tag{1.3}$$

<sup>1)</sup>The Coulomb interaction energy of the electrons  $U_{int} \rightarrow \infty$  as  $R \rightarrow \infty$  since the number  $N$  of electrons interacting with a given electron is proportional to the volume,  $\propto R^3$ , but the interaction energy  $U_{int} N/R \propto R^2$ . However, this term is cancelled by the interaction of the electrons with the nuclei and of the nuclei among themselves. In the spherical approximation this cancellation is exact. However, here the intracellular part of the Coulomb interaction energy of the electrons is large.

Table I

$\mu$	$E_{F0}^+(\mu)$	$E_{F0}^-(\mu)$	$\Delta E_{F0}(\mu)$	$E_{F\mu}^+(\mu)$	$E_{F\mu}^-(\mu)$	$\Delta E_{F\mu}(\mu)$
0	-0.1054	-0.1054	0	-0.1054	-0.1054	0
2	-0.1407	-0.2361	+0.0954	-0.1454	-0.2411	+0.0957
3	-0.1090	-0.2542	+0.1444	-0.1070	-0.2506	+0.1435

In the symbol  $E_{F\mu}^{\pm}(\mu)$  the argument  $\mu$  reflects the dependence of  $E_F$  on the state with respect to  $\mu$  for the given bands  $E(\mu)$ , and the subscript  $\mu$  reflects the dependence on the occupation of the very same bands  $E(\mu)$ . The direct calculation by Podval'nyi for Fe showed that the difference  $E_{F\mu}^+ - E_{F\mu}^-$  essentially does not depend on the subscript  $\mu$  (see Table I; the values of  $E_{F\mu}^{\pm}$  are in atomic units of energy).

Thus, instead of (1.3) we obtain

$$E_H(\mu) - E_H(0) \approx \int_0^{\mu} [E_{F0}^+(\mu) - E_{F0}^-(\mu)] N d\mu.$$

In other words,

$$E_H(\mu) - E_H(0) \approx E_H'(\mu) - E_H'(0), \quad (1.4)$$

where

$$E_H'(\mu) \equiv \sum_{E_i < E_F^+} E_i + \sum_{E_i < E_F^-} E_i,$$

and the  $E_i$  are the Hartree eigenvalues calculated for the nonmagnetic ( $\mu = 0$ ) state. Since  $E_{ex}$  changes markedly upon a change of the occupation, then the small relative error in it associated with the replacement of  $\psi_H(\mu)$  by  $\psi_H(0)$  is unimportant.

## 2. PRACTICAL CALCULATION OF THE ENERGY

One can characterize the eigenfunctions of the electrons in a crystal by the values of the quasimomentum  $\mathbf{k}$  and by a band index  $\nu$  which takes a finite number of values. Changing to an infinite crystal and referring the energy to a single cell, we obtain

$$E_{HF}(\mu) - E_{HF}(0) \approx E_{HF}'(\mu) - E_{HF}'(0), \quad E_{HF}' = E_{HF}^+ + E_{HF}^-,$$

$$E_{HF}^{\pm} = \sum_{\nu} \int_{E_{k\nu} < E_F^{\pm}} E_{k\nu} \frac{d\mathbf{k}}{\omega_k} - \frac{1}{2} \int_{\omega} d\mathbf{r} \int_{\infty} d\mathbf{r}' \frac{|\rho_{\pm}(\mathbf{r}|\mathbf{r}')|^2}{|\mathbf{r} - \mathbf{r}'|}, \quad (2.1)$$

where  $\omega$  is the volume of the cell,  $\omega_k = (2\pi)^3/\omega$  =  $4\pi k_0^3/3$  is the volume of the first Brillouin zone,

$$\rho_{\pm}(\mathbf{r}|\mathbf{r}') \equiv \sum_{\nu} \int_{\pm} \frac{d\mathbf{k}}{\omega_k} \Psi_{k\nu}^*(\mathbf{r}') \Psi_{k\nu}(\mathbf{r})$$

are the electron densities, where the functions  $\Psi_{k\nu}$  are assumed to already be normalized in the cell  $\omega$ . The limiting energies  $E_F^{\pm}$  are determined from the conditions

$$\sum_{\nu} \int_{E_{k\nu} < E_F^{\pm}} \frac{d\mathbf{k}}{\omega_k} = \frac{1 \pm \mu}{2}. \quad (2.2)$$

Since expression (2.1) now no longer leads to small differences between large quantities in (1.1), then in the expressions for  $E'$  and  $\rho_{\pm}$  one can retain only the terms pertaining to unfilled bands: the remaining terms give practically no contribution to (1.1). The intercellular part of the exchange energy in (2.1) (i.e., the case when  $\mathbf{r}$  and  $\mathbf{r}'$  lie in different cells) can be estimated, for example, as indicated in<sup>[5]</sup>. For the 3d-band of Fe

it amounts to not more than 6% of the intracellular part. In fact, Wohlfarth has conjectured that the correlation effects strongly decrease the intracellular part and thereby primarily promote the intercellular part.

However, apparently the actual situation is just the opposite.<sup>[6]</sup> We shall not go into a detailed discussion of this question here since it falls outside the scope of the HF approximation in which our calculations are being done. In what follows we shall confine our attention to the intracellular part of the exchange energy in (2.1)

$$E_{ex}^{\pm} = -\frac{1}{2} \iint_{\omega} \frac{|\rho_{\pm}(\mathbf{r}|\mathbf{r}')|^2}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r} d\mathbf{r}'. \quad (2.3)$$

In the spherical approximation the only direction in the cell which is singled out is the direction of  $\mathbf{k}$ . Therefore, each eigenfunction corresponds to a definite value  $m$  for the component of the electron's angular momentum along  $\mathbf{k}$ , and since there is no preferred direction of rotation, then degeneracy exists with respect to the sign of  $m$ . In particular, in the spherical approximation the d-band which we are interested in splits up into three sub-bands (instead of five in the actual lattice) corresponding to  $m = 0, \pm 1, \pm 2$ . For  $\mathbf{k} = 0$  they all merge into a single point (instead of three sub-bands merging into one point and the other two sub-bands merging into a different point, which occurs in a lattice having cubic symmetry). Thus, one can denote the eigenfunctions  $\Psi_{\mathbf{k}\nu}$  by  $\Psi_{\mathbf{k}m}$  (since we are only interested in the d-band) and represent them in the form

$$\Psi_{\mathbf{k}m}(\mathbf{r}) = \sum_{l \geq |m|} i^l A_{\mathbf{k}|m|l} R_{Bl}(r) \frac{1}{\sqrt{4\pi}} Y_{lm}^{\mathbf{k}}(\mathbf{r}^0),$$

where  $E \equiv E_{\mathbf{k}} |m|$  and  $Y_{lm}^{\mathbf{k}}(\mathbf{r}^0)$  are the spherical harmonics whose polar angle is measured from  $\mathbf{k}$ . The factor  $i^l$ , as it turns out, makes it possible to assume the coefficients  $A_{\mathbf{k}|m|l}$  to be real for real  $R_{Bl}(r)$ .

It is obvious that  $A_{\mathbf{k}|m|l}$  and  $E_{\mathbf{k}} |m|$  depend on the magnitude of the vector  $\mathbf{k}$  and on the number  $m$ . In our calculations the functions  $R(r)$  and  $Y_{lm}$  are normalized according to the conditions

$$\int_0^{r_0} R_{Bl}^2(r) r^2 dr = 1, \quad \int |Y_{lm}|^2 \frac{d\mathbf{r}^0}{4\pi} = 1$$

( $r_0$  denotes the radius of the cell in units of the Bohr radius). Then from the normalization condition on  $\Psi_{\mathbf{k}m}$  it follows  $\sum_l |A_{\mathbf{k}|m|l}|^2 = 1$ . After integrating over the solid angle  $d\mathbf{k}^0$ , in virtue of the spherical symmetry of the problem only the terms with identical values of  $l$  in  $\Psi_{\mathbf{k}m}^*(\mathbf{r}')$  and  $\Psi_{\mathbf{k}m}(\mathbf{r})$  give a nonvanishing contribution to  $\rho_{\pm}(\mathbf{r}|\mathbf{r}')$  so that we obtain

$$\rho_{\pm}(\mathbf{r}|\mathbf{r}') = \sum_{m, l \geq |m| \pm} \int \frac{3k^2 dk}{4\pi k_0^3} A_{\mathbf{k}|m|l}^2 R_{Bl}(r') R_{Bl}(r) P_l(r^0 r'^0), \quad (2.4)$$

where  $P_l$  is the unnormalized Legendre polynomial. If one sets  $\mathbf{r} = \mathbf{r}'$  in (2.4) then, taking into consideration

that  $P_l(1) = 1$ , we obtain the natural expression for the change density:

$$\rho_{\pm}(r) = \sum_{m, l \geq |m|} \int_{\pm} \frac{3k^2 dk}{4\pi k_0^3} A_{k|ml}^2 R_{El}^2(r).$$

In order to take the degeneracy with respect to the sign of  $m$  into account, we introduce the coefficient

$$\delta_m = \begin{cases} 1, & m = 0 \\ 2, & m \neq 0 \end{cases}.$$

Then instead of (2.4) we finally obtain

$$\rho_{\pm}(r|r') = \sum_{l, m \geq 0} \delta_m P_l(r^0 r'^0) \int_{\pm} \frac{3k^2 dk}{4\pi k_0^3} A_{k|ml}^2 R_{El}(r') R_{El}(r). \quad (2.5)$$

Let us expand the product  $P_l P_{l'}$  in the expression for  $|\rho_{\pm}(r|r')|^2$  in terms of Legendre polynomials:<sup>[7]</sup>

$$P_l(\cos \theta) P_{l'}(\cos \theta) = \sum_{L=|l-l'|}^{l+l'} \langle K_{l'l'0}^{L0} \rangle^2 P_L(\cos \theta);$$

here the  $K_{l'l'0}^{L0}$  are the coefficients for the vector addition of angular momenta. In particular, the most important (Coulomb) coefficient for  $L = 0$  is  $(K_{l'l'0}^{00})^2 = \delta_{ll'} / (2l + 1)$ . Still keeping in mind the expansion of  $1/|\mathbf{r} - \mathbf{r}'|$  in terms of Legendre polynomials, instead of expression (2.3) we obtain

$$E_{\text{ex}}^{\pm} = - \sum_{m, m' \geq 0} \delta_m \delta_{m'} \sum_{\substack{l > m \\ l' > m'}}^{\frac{k_{\text{Fm}}^{\pm}}{k_0^3}} \int_0^{\frac{k_{\text{Fm}}^{\pm}}{k_0^3}} \frac{3k^2 dk}{k_0^3} A_{kml}^2 \int_0^{\frac{k_{\text{Fm}}^{\pm}}{k_0^3}} \frac{3k'^2 dk'}{k_0^3} A_{k'm'l'} \times \sum_L \frac{1}{2L+1} (K_{l'l'0}^{L0})^2 \int_0^{r_0} R_{El}(r) R_{E'l'}(r) r dr \int_0^r R_{El}(r') R_{E'l'}(r') r'^2 \left(\frac{r'}{r}\right)^L dr'. \quad (2.6)$$

According to<sup>[2]</sup> the 4s band in the Fe group and the 5s band in the Pd group are filled. Therefore we shall not consider the interaction of these bands with the d-bands, but we shall confine our attention to an investigation of the interaction only inside the d-band. In the calculation of the energy bands, terms with  $0 \leq l \leq 7$  were taken into account; however, the calculation of the energy was carried out taking only  $l = 1, 2$ , and 3 into account. As will be seen, the remaining terms are small for the d-band.

The next appreciable simplification of (2.6) is achieved by neglecting the dependence of  $R_{El}(r)$  on the electron's energy in the d-band. From Fig. 1 it is clear that for  $l = 1, 3$  the energy dependence of  $R_{El}(r)$  is weak (the two graphs for a given  $l$  correspond to the beginning and end of the energy band), but for  $l = 2$  the energy dependence is rather important. This is natural since the width of the d-band is exactly determined by the energy dependence for  $l = 2$ . In our calculations, however, for all three values  $l = 1, 2$ , and 3 the functions  $R_{El}(r)$  were taken for an average value of the energy in the d-band.

This approximation was carried out for Fe and V where only the main terms corresponding to  $l = l' = 2$  and  $L = 0$  were taken into consideration in the calculations. Taking the energy dependence of  $R_{El}(r)$  into account with the aid of an interpolation formula led to a change  $\Delta E_{\text{ex}}$  which was smaller than 5% of its initial value. It is clear that a displacement of the function  $R_{El}(r)$  to the edges of the band can now lead to an appreciable change  $\Delta E$ , which one must keep in mind in

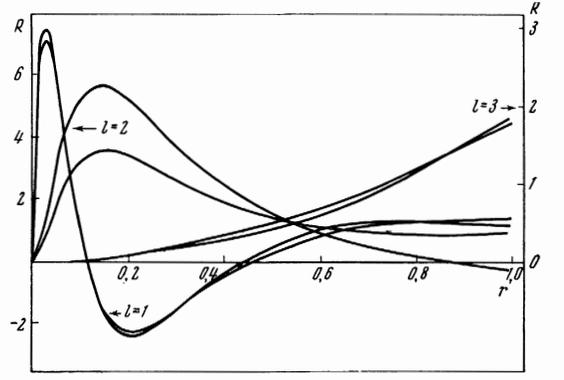


FIG. 1. The functions  $R(r)$ . Values of  $r$  are given in units of  $r_0$ , and of  $R$  in units of  $(1/r_0)^{3/2}$ . The scale for  $l = 3$  is 2.5 times larger than for  $l = 1, 2$ .

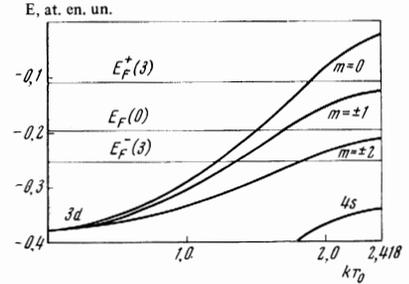
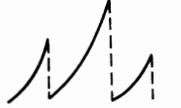


FIG. 2. Graph of the Functions  $E(kr_0)$  for Fe.

FIG. 3. Qualitative Dependence of  $\Delta N/\Delta E$  on  $E$ .



connection with more accurate calculations. If we assume that  $R_{El}(r)$  does not depend on the energy, then (2.6) takes the form

$$E_{\text{ex}}^{\pm} = - \sum_{ll'} N_{l'l'}^{\pm}(\mu) N_{l'l'}^{\pm}(\mu) I_{ll'}, \quad (2.7)$$

where

$$N_{l'l'}^{\pm}(\mu) = \sum_m \int_0^{\frac{k_{\text{Fm}}^{\pm}}{k_0^3}} \frac{3k^2 dk}{k_0^3} A_{kml}^2, \\ I_{ll'} = \int_0^{r_0} R_l(r) R_{l'}(r) r dr \int_0^r R_l(r') R_{l'}(r') r'^2 \left(\frac{r'}{r}\right)^L dr'.$$

We present the values of the coefficients:

$$I_{11} = 1 \cdot \frac{1}{3} I_{11}^0 + \frac{1}{5} \cdot \frac{2}{3} I_{11}^2, \quad I_{12} = \frac{1}{3} \cdot \frac{2}{5} I_{12}^1 + \frac{1}{7} \cdot \frac{3}{5} I_{12}^3, \\ I_{13} = \frac{1}{5} \cdot \frac{9}{21} I_{13}^2 + \frac{1}{9} \cdot \frac{4}{7} I_{13}^4, \\ I_{22} = 1 \cdot \frac{1}{5} I_{22}^0 + \frac{1}{5} \cdot \frac{2}{7} I_{22}^2 + \frac{1}{9} \cdot \frac{18}{35} I_{22}^4, \\ I_{23} = \frac{1}{3} \cdot \frac{9}{35} I_{23}^1 + \frac{1}{7} \cdot \frac{4}{15} I_{23}^3 + \frac{1}{11} \cdot \frac{10}{21} I_{23}^5, \\ I_{33} = 1 \cdot \frac{1}{7} I_{33}^0 + \frac{1}{5} \cdot \frac{4}{21} I_{33}^2 + \frac{1}{9} \cdot \frac{18}{77} I_{33}^4 + \frac{1}{13} \cdot \frac{100}{231} I_{33}^6.$$

### 3. RESULTS OF THE CALCULATIONS

According to the results of article<sup>[2]</sup> the 3-d bands have the shape shown in Fig. 2. The structure of the

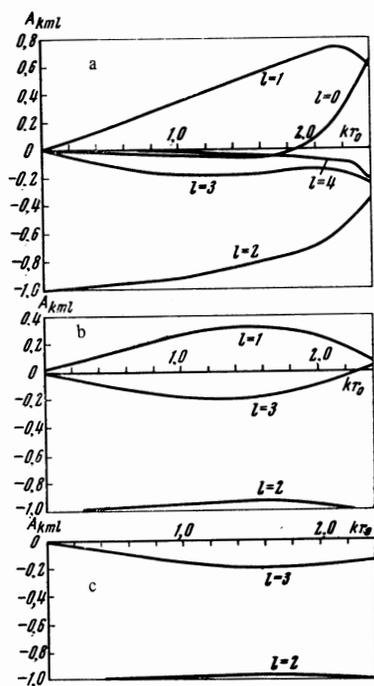


FIG. 4. Dependence of  $A_{kml}$  on  $kr_0$  for the following cases: a— $m = 0$ , b— $m = \pm 1$ , and c— $m = \pm 2$ .

sub-bands for the remaining metals V, Ni, Nb, Ru, and Pd is qualitatively the same. It is clear that the 4s band in the Fe group and the 5s band in the Pd group are always filled so that the number of d-electrons is equal to 3 for V and Nb, it is equal to 6 for Fe and Ru, equal to 8 for Ni and Pd, and equal to 9 for Cu, and the maximum possible magnetic moments per atom are equal, respectively, to  $3 = 3 - 0$ ,  $4 = 5 - 1$ ,  $2 = 5 - 3$ , and  $1 = 5 - 4$  Bohr magnetons.

This band structure leads to an energy dependence for the density of electron states which is qualitatively described by the picture shown in Fig. 3, and which is the same for all of the metals under consideration. The infinite discontinuities correspond to complete occupation of the sub-bands with  $m = \pm 2, \pm 1, 0$ , respectively. This is associated with the fact that the curve  $E_m(k)$  has a maximum near the boundary of the corresponding sub-band. In the real bands, i.e., corresponding to the true crystal lattice, the curve smoothes out, and the density of states vanishes at the boundaries of the d-band. This property may substantially change our results, especially the saturation value of the magnetic moment which is determined in the neighborhood of the band boundary. On the other hand, this apparently does not touch upon the most interesting question concerning the pseudo-magnetism of V, since for nonmagnetic V the Fermi surface occurs far away from the band boundary. Although the d-band is being considered and therefore, for  $k = 0$ , only the terms with  $l = 2$ ,  $A_0 |m| = 1$  for all  $m$  enter into the eigenfunctions, this is not so for  $k \neq 0$ , and for the sub-band  $m = 0$  with large values of  $k$  the terms with  $l = 0, 1$  give the major contribution, that is, the d-states go over into s- and p-states. The terms with  $l = 2$  (see Fig. 4) always give the major contribution for the values  $m = \pm 1, \pm 2$ .

Table II

$\mu$ \ N	$N_{1+}$	$N_{2+}$	$N_{3+}$	$N_{1-}$	$N_{2-}$	$N_{3-}$	$N$
0	0.1020	2.7840	0.0857	0.1020	2.7840	0.0857	5.9434
1	0.1622	3.2075	0.0951	0.0679	2.3376	0.0731	5.9434
2	0.2000	3.6613	0.0979	0.0527	1.8727	0.0600	5.9446
3	0.2466	4.1075	0.1005	0.0367	1.4100	0.0449	5.9462
4	0.4822	4.2650	0.1177	0.0211	0.9474	0.0278	5.8612

Table III

$\mu$	$\Delta E_{ex}(\text{Fe})$	
	$l = 0, 1, 2, 3$	$l = 2$
3	-0.3454	-0.3331
3.5	-0.3901	-0.3606
4	-0.3914	-0.3395

Table IV

Element	$\mu$	$\Delta E_d$	$\Delta E_{ex}$	$\Delta E$
V	1	+0.0122	-0.0274	-0.0152
	2	+0.0505	-0.1105	-0.0600
	3	+0.1225	-0.2419	-0.1194
Fe	1	+0.0186	-0.0240	-0.0054
	2	+0.0585	-0.1408	-0.0823
	3	+0.1129	-0.3331	-0.2202
	4	+0.2156	-0.3395	-0.1239
Ni	0,5	+0.0010	-0.0179	-0.0169
	1,0	+0.0059	-0.0320	-0.0261
	1,5	+0.0258	+0.0065	+0.0323
Nb	2,0	+0.0580	+0.0864	+0.1444
	1	+0.0146	-0.0184	-0.0038
Ru	2	+0.0599	-0.0740	-0.0141
	3	+0.1462	-0.1427	-0.0065
	1	+0.0267	-0.3223	+0.0044
Pd	2	+0.1004	-0.0954	+0.0150
	3	+0.1928	-0.1828	+0.0100
	4	+0.3442	-0.1285	+0.2157
	0,4	+0.0003	-0.0077	-0.0074
Pd	0,8	+0.0038	-0.0041	-0.0003
	1,0	+0.0103	+0.0125	+0.0228
	1,4	+0.0410	+0.0539	+0.0949
	2,0	+0.0951	+0.1438	+0.2389

The coefficients  $A_{kml}$  lead to the effective numbers  $N_l^{\pm}$  of electrons for Fe cited in Table II. The difference between the values of  $N$  and 6 corresponds to the contributions from  $l = 0$  and  $l \geq 4$ .

The total widths of the d-bands are given by the following:

Element:	V	Fe	Ni	Nb	Ru	Pd
Width:	0.3259	0.3392	0.2894	0.3515	0.4457	0.3576

The exchange integrals (see Eq. (2.6) for Fe are given by

$I_{11}^0$	$I_{11}^2$	$I_{13}^1$	$I_{12}^3$	$I_{13}^4$	$I_{13}^4$	$I_{22}^0$	$I_{22}^2$
0.2184	0.1364	0.0383	0.0361	0.1477	0.1203	0.4102	0.1871
$I_{22}^4$	$I_{22}^1$	$I_{22}^3$	$I_{22}^5$	$I_{33}^0$	$I_{33}^2$	$I_{33}^4$	$I_{33}^6$
0.1157	0.0407	0.0271	0.0202	0.2318	0.1806	0.1480	0.1254

The values obtained for  $I_{22}$  are cited below:

Element:	V	Fe	Ni	Nb	Ru	Pd
$I_{22}$ :	0.0714	0.0993	0.1136	0.0535	0.0708	0.0723

It is clear that by virtue of the smallness of the number of electrons for  $l \neq 2$  and by virtue of the insignificant nature of the exchange integrals connecting the states  $l = 0, 1, 3$  with the states  $l = 2$ , one can restrict attention to  $l = 2$ . In particular, the data cited in Table III was obtained for Fe.

The results of calculations taking into account only states with  $l = 2$  are cited in Table IV.

On account of the transition of d-states into s- and p-states near the band boundaries, the effective number of electrons  $N_2^+$  associated with the transition from  $\mu = 3$  to  $\mu = 4$  increases slightly, which leads to a loss in energy. Therefore, the saturation value of the magnetic moment for Fe is found to be  $\mu \approx 3$  (the experimental value is  $\mu \approx 2.2$ ). This difference may be associated, for example, with the spherical approximation. For Ni one obtains  $\mu \approx 0.8$  instead of the experimental value  $\mu \approx 0.6$ , and Cu turns out to be nonmagnetic in general.

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