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Density of States of Conduction Electrons in Ferromagnetic Materials

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The topic of state density of conduction electrons in ferromagnetic metals is considered in the limits of the model of interacting external and internal electrons of the ferromagnetic material.

KNOWLEDGE of the density of levels of valence electrons in metals is very important for the study of soft emission and absorption x-ray spectra of metals. On the other hand, from the study of the fine structure of the edge of the absorption band one can hope to get detailed information concerning the higher energy levels of the electrons in the metals.

Theoretical studies of this subject were formerly made on the basis of the single electron zonal theory of metals, which neglects the electron interaction. However, in the case of ferromagnetic metals, the electrons of which represent a united and a strongly interacting quantum system, study of this problem in the limits of the one electron model is without meaning, since ferromagnetism itself depends on interaction among the electrons.

For the generalization of the calculation of the density of states[1] in the case of ferromagnetic materials let us use a model of exchange interaction of external *s*-electrons and internal *d*-electrons as suggested by Vonsovskii[2,3]. This model has enabled us to understand the nature, and give the quantitative explanation, of "anomalies" of electrical, optical, galvanomagnetic and thermomagnetic properties of ferromagnetic metals [4-11]. According to this model we will consider the system of *s*-electrons in ferromagnetic metals as a mixture of two electron "gases" with two corresponding possible spin orientations. The energy of *s*-electrons in the approximation of effective mass is equal to

$$E = \alpha - \alpha' y\vec{\sigma} + (\beta + \beta' y\vec{\sigma})\mathbf{k}^2, \qquad (1)$$

where a, a', β and β'- are the parameters depending on the exchange integrals of the *s* and *d*-electrons and the translation integrals of the *s*-electron, y is the average relative atomic magnetic moment of the *d*-electron, $\vec{\sigma}$ is the spin vector of the *s*-electron and k is the quasimomentum of the electron. It is seen from Eq. (1) that the effective mass is equal to

$$m_{\pm} = \hbar^2/2a^2(\beta \pm \beta' y), \qquad (2)$$

where the positive sign corresponds to right hand, and the negative to left hand, spin orientations, and *a* is the lattice constant.

According to the zonal theory of metals the expression for the density of states is as follows [1] :

$$n(E) = \pm 2\frac{m^2}{8\pi^3\hbar^4|g|} \qquad (3)$$

$$\times \int_{-E_g}^{E - V_{000} - E_g} \frac{\Gamma d\Gamma}{\sqrt{\Gamma^2 - |V_g|^2}},$$

where E is the energy of the electron in the metal, $E_g = (\hbar^2/2m)\pi^2 g^2$ is the kinetic energy of an electron, which is moving in a direction perpendicular to the reflecting lattice and undergoing Bragg

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[1] A. Wilson, *Quantum Theory of Metals*, 1941, pp. 42-44

[2] S. V. Vonsovskii, J. Exper. Theoret. Phys. USSR **16**, 981 (1946)

[3] S. V. Vonsovskii and E. A. Turov, J. Exper. Theoret. Phys. USSR **24**, 419 (1953)

[4] S. V. Vonsovskii, J. Exper. Theoret. Phys. USSR **18**, 219 (1948)

[5] S. V. Vonsovskii, Izv. Akad. Nauk SSSR, Ser. Fiz. **11**, 463 (1947)

[6] S. V. Vonsovskii and A. V. Sokolov, J. Exper. Theoret. Phys. USSR **19**, 615,703 (1949)

[7] S. V. Vonsovskii and A. V. Sokolov, Doklady Akad. Nauk SSSR **76**, 197 (1951)

[8] A. V. Sokolov and A. Z. Veksler, Doklady Akad. Nauk SSSR **81**, 27 (1951)

[9] A. V. Sokolov and A. Z. Veksler, J. Exper. Theoret. Phys. USSR **25**, 215 (1953)

[10] S. V. Vonsovskii and K. P. Rodionov, Doklady Akad. Nauk SSSR **75**, 643 (1950)

[11] S. V. Vonsovskii, L. Ja. Kobelev and K. P. Rodionov, Izv. Akad. Nauk SSSR, Ser. Fiz. **16**, 569 (1952)

reflection, V_{000} and V_g are the Fourier coefficients in the expansion of the lattice potential, g is the vector of the inverse lattice and

$$\Gamma = E - V_{000} - E_g - (\hbar^2/2m)(\varkappa_2^2 + \varkappa_3^2);$$

κ_2 and κ_3 are the components of the quasimomentum of the electron parallel to the zone boundary, and the component $\kappa_1' = -\pi|g| + \kappa_1$ is directed parallel to g. The positive sign in Eq. (3) should be taken for the states of the upper band and the negative for the states of the lower band.

In the case of ferromagnetic metals Eq. (1) is replaced by the expressions

$$n_+(E) = \pm \frac{m_+^2}{8\pi^3\hbar^4|g|} \int \frac{\Gamma_+ d\Gamma_+}{\sqrt{\Gamma_+^2 - |V_g|^2}}, \tag{4}$$

$$n_-(E) = \pm \frac{m_-^2}{8\pi^2\hbar^4|g|} \int \frac{\Gamma_- d\Gamma_-}{\sqrt{\Gamma_-^2 - |V_g|^2}}.$$

Note that the limits of integration in Eq. (4) are different from the limits of integration in Eq. (3). Here

$$\Gamma_\pm = \pm \sqrt{|V_g|^2 + \left(1 \pm \frac{\beta'}{\beta} y\right)^2 \left(\frac{\pi\hbar^2 g\varkappa_1}{m}\right)^2}, \tag{5}$$

where $n_+(E)$ is the density of states corresponding to the right hand spin orientation, and $n_-(E)$ to the left hand spin orientation. Thus it is natural to consider as justified the relation

$$n(E, y) = n_+(E, y) + n_-(E, y). \tag{6}$$

By restricting ourselves to a temperature range "close" to the Curie point ($y \ll 1$), one can expand $\Gamma_\pm$ in a power series in y and retain only the terms up to second order. Then we get

$$\Gamma_\pm d\Gamma_\pm = \Gamma d\Gamma \left(1 \pm \frac{\beta'}{\beta} y\right)^2, \tag{7}$$

$$\sqrt{\Gamma_\pm^2 - |V_g|^2} = \left(1 \pm \frac{\beta'}{\beta} y\right) \sqrt{\Gamma^2 - |V_g|^2}. \tag{8}$$

From this it follows that the integrand of Eqs. (4) can be represented as follows:

$$\frac{\Gamma_\pm d\Gamma_\pm}{\sqrt{\Gamma_\pm^2 - |V_g|^2}} = \left(1 \pm \frac{\beta'}{\beta} y\right) \frac{\Gamma d\Gamma}{\sqrt{\Gamma^2 - |V_g|^2}}. \tag{9}$$

Further, we have the obvious relation

$$m_\pm^2 X_\pm = \frac{m_1 \Gamma d\Gamma}{\sqrt{\Gamma^2 - |V_g|^2}} \frac{1}{(1 \pm (\beta'/\beta) y)}, \tag{10}$$

where $X_\pm$ is equal to Eq. (9) and $m_1 = \hbar^2/2a^2\overline{\beta}$ Taking into account Eqs. (4)-(10) we will get for the densities of states of the electrons, n_+ and n_-, the expression

$$n_\pm(E, y) = \pm \frac{m_1^2}{8\pi^3\hbar^4|g|} \frac{1}{(1 \pm (\beta'/\beta) y)} \int \frac{\Gamma d\Gamma}{\sqrt{\Gamma^2 - |V_g|^2}} \tag{11}$$

and, finally, for the total density of states of conduction electrons in ferromagnetic materials the relation:

$$n(E, y) = n_+(E, y) + n_-(E, y) \tag{12}$$

$$\approx \pm \frac{m_1^2}{4\pi^3\hbar^4|g|} (1 + A^2y^2) \int \frac{\Gamma d\Gamma}{\sqrt{\Gamma^2 - |V_g|^2}},$$

where $A = \beta'/\beta$ is not greater than unity. The limits of integration in Eq. (12) are the same as in Eq. (3)

Consider three different energy intervals:

I) $E < V_{000} + E_g - |V_g|$.

All states satisfying this inequality are in the lower band so that the negative sign is used:

$$n(E, y) = (1 + A^2y^2) \frac{m_1^2}{4\pi^3\hbar^4|g|} [(E^2 - |V_g|^2)^{1/2} \tag{13}$$

$$- \{(V_{000} + E_g - E)^2 - |V_g|^2\}^{1/2}].$$

II) $V_{000} + E_g - |V_g| < E < V_{000} + E_g + |V_g|$.

These states are also located in the lower band; however, for the upper limit of Γ here one should use $|V_g|$; then we get:

$$n(E, y) = (1 + A^2y^2) \frac{m_1^2}{4\pi^3\hbar^4|g|} (E_g^2 - |V_g|^2)^{1/2}. \tag{14}$$

III) $V_{000} + E_g + |V_g| < E$.

The states for which Γ is less than $|V_g|$ are in the lower band; the states for which Γ is greater than $|V_g|$ are in the upper band:

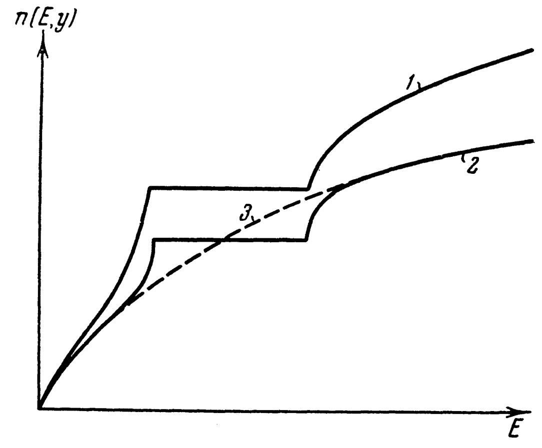
$$n(E, y) = (1 + A^2y^2) \frac{m_1^2}{4\pi^3\hbar^4|g|} \tag{15}$$

$$\times \left[- \int_{-E_g}^{-|V_g|} + \int_{|V_g|}^{E - V_{000} - E_g} \right] \frac{\Gamma d\Gamma}{(\Gamma^2 - |V_g|^2)^{1/2}}$$

$$= (1 + A^2y^2) \frac{m_1^2}{4\pi^3\hbar^4|g|} [(E_g^2 - |V_g|^2)^{1/2}$$

$$+ \{(E - E_g - V_{000})^2 - |V_g|^2\}^{1/2}].$$

The functions $n(E,y)$ and $n(E,O)$ are plotted in the Figure [$n(E,O)$ is $n(E,y)$ at $y = 0$].



1-curve of $n(E,y)$
2-curve of $n(E,O)$
3-n for free electrons

Notice that the deviation of the curves for $n(E,y)$ and $n(E,O)$ from that for free electrons (shown by the dotted line) depends on only two planes, g and -g, while at least six planes should be considered. Hence these deviations should be multiplied by the number of pairs of equivalent planes which bound the lower band.

From Eqs. (12)-(15) and from the Figure one can see that the curve $n(E,y)$ lies above the curve $n(E,O)$. From this it follows that if one were to take into account several equivalent planes, the jump in the density of states $n(E,y)$ of the conduction electrons of the ferromagnetic material close to the Curie temperature would be greater than in the case of no magnetization. At $y = 0$, Eq. (13) is the same as Eq. (3) for the density of states in ordinary metals. It is not hard to see that Eq. (13) can easily be put in the form:

$$n(E, y) = n(E, 0)(1 + A^2y^2). \qquad (16)$$

Notice from this expression that the density of states of conduction electrons of ferromagnetic materials is a quadratic function of spontaneous magnetization. The spontaneous magnetization is a function of temperature, as a consequence of which the density value of electron states in the ferromagnetic material, which depends on y, must show anomalous temperature dependence. Since the intensities of x-ray spectral lines (as well as the corresponding transition probabilities) are proportional to the densities of the electron states, these intensities for ferromagnetic metals will also show anomalous temperature dependences.

An increase of magnetization, as Eqs. (12)-(16) show, increases the density of states of the conduction electrons in a ferromagnetic material. This permits us to conclude that the band of s-electron levels of a ferromagnetic material becomes narrower. This conclusion is in agreement with the fact that in a ferromagnetic material to a first approximation the spins of the d-electron system are strongly bound among each other, the orbital moments cancel each other and a phenomenon analogous to the Paschen-Bach effect takes place. In other words, under the influence of a strong internal "magnetic field", caused by the exchange interaction of the s and d-electrons a simplification of the picture of levels of the s-electron system (narrowing of the band) occurs rather than a complication.

From Eq. (16) one can easily get an expression for the ferromagnetic "anomaly" of the density of electron states in ferromagnetic materials:

$$\frac{n(E, y) - n(E, 0)}{n(E, 0)} = A^2y^2. \qquad (17)$$

The value of the ferromagnetic "anomaly" of the density of electron states in ferromagnetic material is proportional to the square of the spontaneous magnetization y. It is very desirable to check experimentally the theoretical conclusions represented by Eq. (17).

Hence, by using the exchange model of external and internal electrons of ferromagnetic materials, we have suceeded in showing that the density of electron states in ferromagnetic materials must depend on the spontaneous magnetization. Near the temperature of ferromagnetic transition this dependence is of a simple quadratic nature [Eq. (16)]. In addition the ferromagnetic "anomaly" of the density of electron states in ferromagnetic metals was obtained.

In conclusion, let us point out that the calculations described above are not claimed to provide a quantitative description of densities of states of conduction electrons in ferromagnetic metals, since they were carried out using a simplified model of ferromagnetic materials. Nevertheless, apparently, there is no reason to doubt that qualitative conclusions about the dependence of the density of states of conduction electrons on spontaneous magnetization must be correct.

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