POSSIBILITY OF DISTRIBUTION OF MAGNETIZATION DIRECTIONS IN BAND MODEL OF THIN FILMS

By L. Wojtczak

Institute of Physics, University of Łódź*

And A. Sukiennicki

Institute of Physics, Technical University, Warsaw**

(Received May 24, 1972)

The band model (in the Stoner approximation) of a ferromagnetic thin film is formulated here in the form allowing to discuss the possibility of a distribution of magnetization directions inside the film. It is shown that the one-band Hamiltonian given by Hubbard, for which the Hartree-Fock approximation is applied, leads to magnetization directed along one arbitrarily chosen direction rather than to a distribution of magnetization directions.

The band model of a ferromagnetic thin film [1] is considered here in a form permitting the discussion the possibility of a distribution of magnetization directions determined by the angles ϑ_ν between the magnetization vector of the ν-th layer and z-axis arbitrarily directed with respect to the surface orientation. From the physical point of view the direction of the z-axis is determined by the film anisotropy or the external magnetic field. In this paper however, the determination of the direction of the z-axis is not important because the subject of the present discussion is only the possibility of a distribution of magnetization directions around this axis. The z-axis is assumed to be equivalent to the easy axis.

The distribution of magnetization directions across the film, related to the fixed direction of the z-axis, can be obtained by minimizing the free energy with respect to ϑ_ν. The thermodynamic functions of the sample with a distribution of magnetization directions can be calculated by a self-consistent method assuming that the eigenstates depend on this distribution.

* Address: Instytut Fizyki, Uniwersytet Łódzki, Narutowicza 68, 90-136 Łódź, Poland.
** Address: Instytut Fizyki, Politechnika Warszawska, Koszykowa 75, 00-662 Warszawa, Poland.

The one-band Hubbard's Hamiltonian applied to thin films [1] with an anisotropic interaction energy term [2] in the sense of the Hartree-Fock approximation can be written as

$$\mathcal{H} = \sum_{\langle \vec{j}\nu\vec{j}'\nu'\rangle m} H\binom{\nu'\vec{j}'}{\nu\vec{j}} C^{+}_{\nu\vec{j}m} C^{-}_{\nu'\vec{j}'m} + \tfrac{1}{2} I \sum_{\nu\vec{j}m} \langle n_\nu \rangle C^{+}_{\nu\vec{j}m} C^{-}_{\nu\vec{j}m} +$$

$$-\tfrac{1}{2} I \sum_{\nu\vec{j}} \langle r_\nu \rangle \left(C^{+}_{\nu\vec{j}\uparrow} C^{-}_{\nu\vec{j}\uparrow} - C^{+}_{\nu\vec{j}\downarrow} C^{-}_{\nu\vec{j}\downarrow}\right) \tag{1}$$

where $C^{\pm}_{\nu\vec{j}m}$ denote the creation and annihilation operators for an electron with the spin $m = \uparrow(\downarrow)$ at the point $\vec{j}$ in the layer ν respectively. I is the intra-atomic Coulomb integral and the $H\binom{\nu'\vec{j}'}{\nu\vec{j}}$, determined in [3], are related to the matrix elements of the electronic potential in the Wannier representation. The symbol $\langle n_\nu \rangle$ denotes the mean number of electrons per atom in the ν-th layer and the $\langle r_\nu \rangle$ is a parameter describing the average magnetic order in the ν-th layer; it corresponds to the spontaneous magnetization per atom in the Stoner approximation.

Assuming a distribution of magnetization directions, the Hamiltonian (1) can be expressed by the new operators $b^{\pm}_{\nu\vec{j}m}$ determined by the relations [4]

$$C^{\pm}_{\nu\vec{j}m} = m \cos\frac{\vartheta_\nu}{2} b^{\pm}_{\nu\vec{j}m} + \sin\frac{\vartheta_\nu}{2} b^{\pm}_{\nu\vec{j}(-m)}. \tag{2}$$

The diagonalization of this Hamiltonian is assured by the following transformation

$$b^{\pm}_{\nu\vec{j}m} = \frac{1}{\sqrt{N}} \sum_{\tau\vec{h}} e^{\pm i\vec{h}\vec{j}} T^{m}_{\nu\tau} b^{\pm}_{\tau\vec{h}m} \tag{3}$$

where $T^{m}_{\nu\tau}$ are the amplitudes of perpendicular electronic waves. N is the number of atoms in a layer.

Our calculations are limited to the case of the absolute zero temperature. The free energy is reduced to the thermodynamic average value of the Hamiltonian (1) taken in the representation (3). The eigenstates $b^{+}_{\tau\vec{h}m}|0\rangle$ form a set of orthonormal eigenvectors. This implies that

$$\langle b^{+}_{\nu\vec{j}m} b^{-}_{\nu'\vec{j}'m'} \rangle_{T=0} = \frac{1}{N} \sum_{\tau\vec{h}} (T^{m}_{\nu\tau} T^{m'}_{\nu'\tau}) e^{i\vec{h}(\vec{j}'-\vec{j})} \delta_{mm'} \langle b^{+}_{\tau\vec{h}m} b^{-}_{\tau\vec{h}m} \rangle_{T=0} \tag{4}$$

and

$$\langle C^{+}_{\nu\vec{j}m} C^{-}_{\nu'\vec{j}'m} \rangle_{T=0} = \cos\frac{\vartheta_\nu}{2} \cos\frac{\vartheta_{\nu'}}{2} \langle b^{+}_{\nu\vec{j}m} b^{-}_{\nu'\vec{j}'m} \rangle_{T=0} +$$

$$+\sin\frac{\vartheta_\nu}{2} \sin\frac{\vartheta_{\nu'}}{2} \langle b^{+}_{\nu\vec{j}(-m)} b^{-}_{\nu'\vec{j}'(-m)} \rangle_{T=0}. \tag{5}$$

Applying the formulae (4) and (5) to the Hamiltonian (1) we find for its average value the expression

$$\langle \mathscr{H} \rangle = \frac{1}{N} \sum_{\langle \nu\vec{j}\nu'\vec{j}' \rangle} \sum_{\tau\vec{h}m} (T^m_{\nu\tau} T^m_{\nu'\tau}) 2 \cos \frac{\vartheta_\nu - \vartheta_{\nu'}}{2} H(^{\nu'\vec{j}'}_{\nu\vec{j}}) e^{i\vec{h}(\vec{j}'-\vec{j})} \langle b^+_{\vec{\tau}hm} b^-_{\vec{\tau}hm} \rangle +$$

$$+ I \sum_{\nu\vec{j}} \langle n_\nu \rangle^2 - I \sum_{\nu\vec{j}} \langle r_\nu \rangle_b^2 \cos^2 \vartheta_\nu \tag{6}$$

where $\langle r_\nu \rangle_b$ denotes the magnetization value in the $b^{\pm}_{\nu\vec{j}m}$ representation. It corresponds to the magnetization value obtained in the model with unidirectional magnetization. The mean number of electrons $\langle n_\nu \rangle$ is invariant with respect to the transformation (2). Taking into account that $H(^{\nu\pm1\,\vec{j}}_{\nu\,\vec{j}}) = -B$ [3] and applying the approximate form $\cos \frac{\vartheta_{\nu'} - \vartheta_\nu}{2} =$ $= 1 - \frac{1}{8} (\vartheta_{\nu'} - \vartheta_\nu)^2$ the formula (6) can be rewritten as follows

$$\langle \mathscr{H} \rangle = \langle \mathscr{H} \rangle_0 + \sum_{\nu\vec{j}} B \sum_{\tau m} T^m_{\nu\tau} (T^m_{\nu-1,\tau} + T^m_{\nu+1,\tau}) \tfrac{1}{8} \left(\frac{\Delta\vartheta_\nu}{\Delta\nu} \right)^2 \times$$

$$\times \frac{1}{N} \sum_{\vec{h}} \langle b^+_{\vec{\tau}hm} b^-_{\vec{\tau}hm} \rangle_{T=0} - I \sum_{\nu\vec{j}} \langle r_\nu \rangle_b^2 \cos^2 \vartheta_\nu \tag{7}$$

where $\langle \mathscr{H} \rangle_0$ does not depend on the angles ϑ_ν. Introducing the notation

$$\alpha_\nu = \tfrac{1}{2} B \sum_{\tau m} T^m_{\nu\tau} (T^m_{\nu-1,\tau} + T^m_{\nu+1,\tau}) \frac{1}{N} \sum_{\vec{h}} \langle b^+_{\vec{\tau}hm} b^-_{\vec{\tau}hm} \rangle_{T=0}$$

$$\beta_\nu = I \langle r_\nu \rangle_b^2 \tag{8}$$

we have

$$\langle \mathscr{H} \rangle = \langle \mathscr{H} \rangle_0 + N \sum_\nu \left[\tfrac{1}{4} \alpha_\nu \left(\frac{\Delta\vartheta_\nu}{\Delta\nu} \right)^2 - \beta_\nu \cos^2 \vartheta_\nu \right]. \tag{9}$$

From the condition for the minimum of (9) we can derive the difference equation

$$\tfrac{1}{2} \alpha_\nu \frac{\Delta^2 \vartheta_\nu}{\Delta\nu^2} - \beta_\nu \sin 2\vartheta_\nu = 0 \tag{10}$$

which is equivalent to the Euler equation obtained in the phenomenological theory [5].

The solution of (10) depends on α_ν which can be treated as parameters. This solution can be found for the boundary conditions determined by the behaviour of the magnetic moment at the surfaces. According to the transformations (2) and (3) however, this solution $\vartheta_\nu = \vartheta_\nu(\alpha_\nu)$ influences the diagonalization procedure. As a result of the diagonalization we find that the coefficients $T^m_{\nu\tau}$ depend on α_ν: $T^m_{\nu\tau} = T^m_{\nu\tau}(\alpha_\nu)$. Taking into account the relation (8) we get a set of consistent equations for ϑ_ν and α_ν.

We can take into account the case when the coefficients β_ν, α_ν are positive. Then the equation (10) (or more precisely the minimum of (9)) is satisfied for $\vartheta_\nu = 0$. This corresponds to unidirectional magnetization. It is just the case considered in [1]; taking into account the analytical form of $T^m_{\nu\tau}$ calculated in [1] for unidirectional magnetization we can obtain α_ν from the relation (8) assuring in this manner the selfconsistency of the procedure. It is clear that our solution satisfies the boundary conditions $\vartheta_1 = \vartheta_n = 0$, where n denotes the number of layers in a film. It is possible that other solutions (*e. g.* Bariachtar's type of the solution [5]) correspond to other boundary conditions.

It is interesting to point out that the distribution of angles ϑ_ν arises as a competition between an exchange stiffness and an anisotropy term of the film [6]. In our model the exchange stiffness is a result of the hopping term of the Hamiltonian (1). It means that there is an unfavorable situation for itinerant electrons to change their quantization direction; this is the physical cause of the stiffness. On the other hand, anisotropy is introduced to our model by the Hartree-Fock approximation of the isotropic Hubbard's Hamiltonian [2]. This approximation is equivalent to some kind of a molecular field. The direction of this molecular field is physically induced by an external magnetic field or by the real anisotropy of the film. In our theory this was not taken into account and this is the reason why we obtained unidirectional magnetization along an arbitrarily chosen direction.

From this point of view, the main result of this paper was showing that unidirectional magnetization used in Refs [1] is consistent with the Hamiltonian (1) used in those papers.

We wish to express our sincere thanks to Professor S. Szczeniowski for reading of the manuscript and helpful criticism.

REFERENCES

[1] S. Szczeniowski, L. Wojtczak, *J. Appl. Phys.*, **39**, 1377 (1968); *J. Phys.* **C-1**, 1176 (1971).
[2] L. Wojtczak, A. Sukiennicki, *Phys. Letters*, **41A**, 37 (1972).
[3] L. Wojtczak, *Acta Phys. Polon.*, **36**, 107 (1969).
[4] S. Alexander, G. Herwitz, *Phys. Rev.*, **164**, 642 (1967); M. Kaneyeshi, *JAERI*, **1197**, 64 (1970).
[5] W. G. Bariachtar, W. F. Klepikov, W. L. Sobolev, *Fiz. Tverdogo Tela*, **13**, 1454 (1971).
[6] A. Sukiennicki, R. Świrkowicz, *Acta Phys. Polon.*, **A40**, 251 (1971).