BLOCH WALLS IN ITINERANT MODEL OF FERROMAGNETISM

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The distribution of magnetization directions in ferromagnetic domain walls is obtained from the itinerant electron model of ferromagnetism. The Bloch wall width and the wall energy is calculated in this model. It is shown that some local decrease of magnetization value in a Bloch wall is to be expected. There appears a possibility of a spontaneous appearance of domain structure.

1. Introduction

Distribution of magnetization directions in ferromagnetic domain wall has been mainly treated by means of phenomenological theory [1–3]. This problem has been also considered for the Heisenberg model of ferromagnetism [4, 5]. However, no calculations have been made in this field for the band model of ferromagnetism, in which electrons are not localised but are considered as waves propagating in a periodical potential of a crystallographic lattice. Some conclusions regarding Bloch walls were also obtained for the last model [6–10]; however, they concerned the so-called "stiffness parameter" [6–9] and the change of magnetization value in Bloch walls [10] rather than the distribution of magnetization directions. As a common point of all these papers [6–10] a linear rotation of magnetization in Bloch wall was assumed. It is known, however, that this rotation is certainly nonlinear. The distribution of magnetization directions in Bloch wall can be obtained only if anisotropy energy is taken into account; this anisotropy was neglected in all the papers [6–10].

The purpose of this paper is to calculate the distribution of magnetization directions in Bloch wall from the point of view of the itinerant electron model of ferromagnetism by means of methods analogous to that used in the paper [6].

2. Domain structure

We consider an uniaxial ferromagnetic crystal. We assume that some domain structure exists in this crystal, but we are not interested in the origin of this structure (tendency to reduce a demagnetizing field energy). If uniaxial anisotropy is large enough, as is assumed in the following, we expect that domains have the form of slabs magnetized antiparallelly and

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separated by 180° Bloch walls (Fig. 1). For smaller anisotropy energy, the so-called closure domains appear; we neglect this possibility.

We assume the Z-axis of the coordinate system perpendicular to the Bloch walls and the X-axis along the easy axis of the crystal. Then, the macroscopic magnetization $\boldsymbol{M}$ rotates in Bloch walls constituting an angle φ with the X-axis; this angle depends on one variable z only. In every point of the walls the macroscopic magnetization remains in the XY plane.

3. Energy of the crystal with the domain structure

We assume that the electron wave function in the crystal can be considered as a determinant constructed from one-electron wave functions. Crystal energy is calculated as a sum of the Hartree-Fock energy [6] and the phenomenological anisotropy energy, without any considerations concerning the origin of this anisotropy.

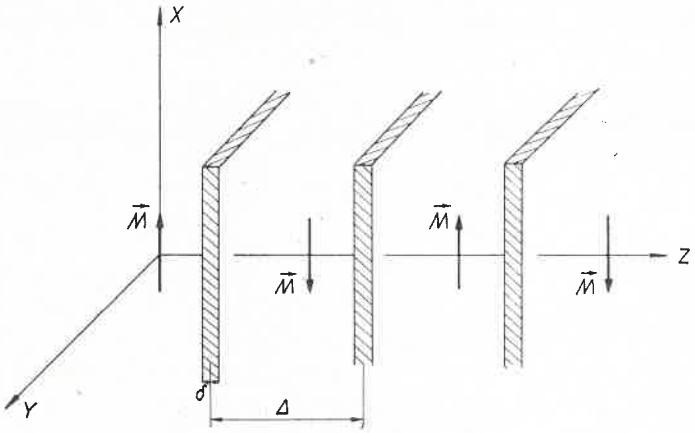

Fig. 1. Domain structure in uniaxial crystal

The ferromagnetic state of a crystal *i. e.* the state in which quantization axes of all electrons are parallel to the X-axis, is described by a determinant constructed from one--electron wave functions of the form

$$\psi_{\boldsymbol{k}}^0 = \chi_{\boldsymbol{k}}^0 g_{\boldsymbol{k}}^0 = \chi_{\boldsymbol{k}}^0 \exp\left(-i\frac{\pi}{4}\sigma_y\right)\begin{pmatrix}1\\0\end{pmatrix}. \tag{1}$$

The energy E_0 of this state in the Hartree-Fock approximation is equal to

$$E_0 = -\frac{\hbar^2}{2m}\sum_{\boldsymbol{k}}\langle \boldsymbol{k}|V^2|\boldsymbol{k}\rangle_0 + \frac{1}{2}\sum_{\boldsymbol{k},\,\boldsymbol{k}'}\langle \boldsymbol{k}\boldsymbol{k}'|G|\boldsymbol{k}\boldsymbol{k}'\rangle_0 - \frac{1}{2}\sum_{\boldsymbol{k},\,\boldsymbol{k}'}\langle \boldsymbol{k}\boldsymbol{k}'|G|\boldsymbol{k}'\boldsymbol{k}\rangle_0, \tag{2}$$

where the subscript 0 means that matrix elements are calculated by means of the states $\psi_{\boldsymbol{k}}^0$; G is the interaction potential between electrons. We introduce a rotation operator $O_{\boldsymbol{k}}$ of the quantization axis of electron with the wave vector $\boldsymbol{k}$ in the following way

$$O_{\boldsymbol{k}} = \exp\left[-\frac{i}{2}\varphi_{\boldsymbol{k}}\sigma_z\right]\exp\left[\frac{i}{2}\left(\frac{\pi}{2}-\vartheta_{\boldsymbol{k}}\right)\sigma_y\right]. \tag{3}$$

This means, that in a state with the domain structure, the quantization axis of this electron is described by spherical angles ϑ_k, φ_k with respect to the Z-axis as the polar axis. The wave function of this state is the determinant from one-electron wave functions of the form

$$\psi_k = \chi_k g_k, \qquad g_k = O_k g_k^0, \tag{4}$$

where χ_k and the angles ϑ_k, φ_k are chosen so as to make the crystal energy

$$E = -\frac{\hbar^2}{2m}\sum_k \langle k|V^2|k\rangle + \frac{1}{2}\sum_{k,\,k'}\langle kk'|G|kk'\rangle - \frac{1}{2}\sum_{k,\,k'}\langle kk'|G|k'k\rangle + E_{\text{anis}} \tag{5}$$

reach the minimum value. The anisotropy energy is introduced here in a phenomenological manner; the density of this energy is equal to

$$\varepsilon_{\text{anis}} = \frac{1}{N}\sum_k K \sin^2 \varphi_k, \tag{6}$$

where N denotes the number of electrons in the crystal (we assume the single occupation of each one of the electron states); K is the uniaxial anisotropy constant assumed the same for all electrons.

By means of (1), (3) the formula (4) leads to

$$\psi_k(r) = e^{ikr}u_k(r)\begin{pmatrix} \exp\left[-i\frac{\varphi_k(r)}{2}\right]\cos\frac{1}{2}\vartheta_k(r) \\ \exp\left[i\frac{\varphi_k(r)}{2}\right]\sin\frac{1}{2}\vartheta_k(r)\end{pmatrix}, \tag{7}$$

where $u_k(r)$ is a periodical function with the crystallographic lattice period.

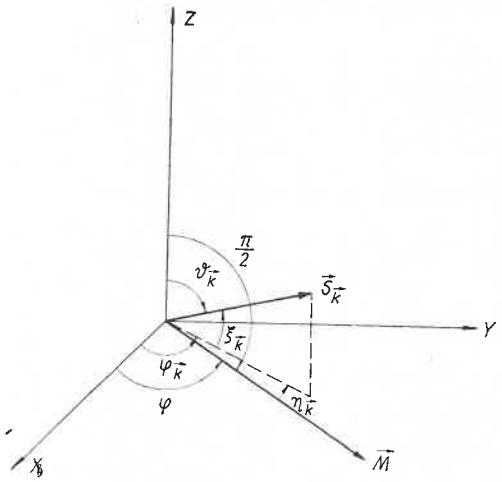

Fig. 2. Quantization axis $\vec{S_k}$ of electron with the wave vector $\vec{k}$, and macroscopical magnetization $\vec{M}$ with respect to the coordinate system

The distribution of electron quantization axes is given by the angles $\vartheta_{\boldsymbol{k}}$, $\varphi_{\boldsymbol{k}}$ or by the angles (Fig. 2)

$$\xi_{\boldsymbol{k}}(\boldsymbol{r}) = \vartheta_{\boldsymbol{k}}(\boldsymbol{r}) - \frac{\pi}{2}, \tag{8}$$

$$\eta_{\boldsymbol{k}}(\boldsymbol{r}) = \varphi_{\boldsymbol{k}}(\boldsymbol{r}) - \varphi(\boldsymbol{r}), \tag{9}$$

where $\varphi(\boldsymbol{r})$ is the angle between the macroscopic magnetization (lying in the XY plane) in the point $\boldsymbol{r}$ and the X-axis. In the following we consider one-dimensional Bloch walls, *i. e.* walls in which all the angles are functions of the one variable z only. It is clear from the definitions that the angles $\xi_{\boldsymbol{k}}$, $\eta_{\boldsymbol{k}}$ constitute the deviation of quantization axis of the electron with wave vector $\boldsymbol{k}$ from the macroscopical magnetization direction which is given by spherical angles $\frac{\pi}{2}$, φ. Therefore, mean values of $\xi_{\boldsymbol{k}}$, $\eta_{\boldsymbol{k}}$ taken with weights $|u_{\boldsymbol{k}}(\boldsymbol{r})|^2$ over elementary cells must be equal to zero if corresponding sums over all occupied electron states are taken:

$$\sum_{\boldsymbol{k}} \int_{\text{e.c.}} d^3r \xi_{\boldsymbol{k}} |u_{\boldsymbol{k}}(\boldsymbol{r})|^2 = 0, \tag{10}$$

$$\sum_{\boldsymbol{k}} \int_{\text{e.c.}} d^3r \eta_{\boldsymbol{k}} |u_{\boldsymbol{k}}(\boldsymbol{r})|^2 = 0. \tag{11}$$

We assume in the following that $\xi_{\boldsymbol{k}}$, $\eta_{\boldsymbol{k}}$ are small and we take into account terms up to the second order with respect to $\xi_{\boldsymbol{k}}$, $\eta_{\boldsymbol{k}}$.

The calculation of the energy terms in the formula (5) by means of methods similar to those in the paper [6] leads to

$$T_{\boldsymbol{kk}} = -\frac{\hbar^2}{2m} \langle \boldsymbol{k}|\nabla^2|\boldsymbol{k}\rangle$$

$$= \frac{\hbar^2}{2m}\left\{\int d^3r |\nabla\chi_{\boldsymbol{k}}|^2 - \frac{i}{2}\int d^3r\, 2\,\mathrm{Re}\,\chi^*_{\boldsymbol{k}}\nabla\chi_{\boldsymbol{k}}\xi_{\boldsymbol{k}}\nabla\varphi_{\boldsymbol{k}} + \frac{1}{4}\int d^3r |\chi_{\boldsymbol{k}}|^2 [|\nabla\varphi_{\boldsymbol{k}}|^2 + |\nabla\xi_{\boldsymbol{k}}|^2]\right\}, \tag{12}$$

$$\langle \boldsymbol{kk}'|G|\boldsymbol{kk}'\rangle = \int d^3r d^3r' |\chi_{\boldsymbol{k}}(\boldsymbol{r})|^2 G(|\boldsymbol{r}-\boldsymbol{r}'|)|\chi_{\boldsymbol{k}'}(\boldsymbol{r}')|^2, \tag{13}$$

$$\langle \boldsymbol{kk}'|G|\boldsymbol{k}'\boldsymbol{k}\rangle = \int d^3r d^3r' G(|\boldsymbol{r}-\boldsymbol{r}'|)\chi^*_{\boldsymbol{k}'}(\boldsymbol{r})\chi_{\boldsymbol{k}'}(\boldsymbol{r}')(g_{\boldsymbol{k}'}(\boldsymbol{r}), g(\boldsymbol{r}))\times$$
$$\times\chi^*_{\boldsymbol{k}}(\boldsymbol{r}')\chi_{\boldsymbol{k}}(\boldsymbol{r})(g_{\boldsymbol{k}}(\boldsymbol{r}'), g_{\boldsymbol{k}'}(\boldsymbol{r}')), \tag{14}$$

$$E_{\text{anis}} = \sum_{\boldsymbol{k}} E^{(k)}_{\text{anis}}, \qquad E^{(k)}_{\text{anis}} = \frac{1}{N}\int d^3r K \sin^2\varphi_{\boldsymbol{k}}, \tag{15}$$

where

$$(g_{\boldsymbol{k}'}(\boldsymbol{r}), g_{\boldsymbol{k}}(\boldsymbol{r})) = 1 - \frac{i}{4}(\eta_{\boldsymbol{k}'} - \eta_{\boldsymbol{k}})(\xi_{\boldsymbol{k}'} + \xi_{\boldsymbol{k}}) - \frac{1}{8}(\eta_{\boldsymbol{k}'} - \eta_{\boldsymbol{k}})^2 - \frac{1}{8}(\xi_{\boldsymbol{k}'} - \xi_{\boldsymbol{k}})^2. \tag{16}$$

The total energy (5) is a function of $\chi_k(\boldsymbol{r})$, $\vartheta_k(\boldsymbol{r})$, $\varphi_k(\boldsymbol{r})$, which have to be chosen so that the total energy takes the minimum value. It is easy to show in the lowest approximation that for this minimum $\chi_k = \chi_k^0$, because each change of χ_k causes an increase of energy. On the other hand, $\xi_k(\boldsymbol{r})$ and $\varphi_k(\boldsymbol{r})$ have to be obtained by means of a variational procedure with the additional condition (10). Next, we can obtain $\varphi(\boldsymbol{r})$ from the formula (11) changed to the form

$$\sum_k \int_{\text{e.c.}} |u_k(\boldsymbol{r})^2[\varphi_k(\boldsymbol{r})-\varphi(\boldsymbol{r})]d^3r = 0. \tag{17}$$

Our problem is a very complicated one in the general case. We solve it in the most crude approximations, in which electrons in a crystal are treated as: (1) gas of electrons interacting by means of screened interactions of delta function type (vanishing range of interaction), (2) gas of electrons with pure Coulomb interactions (long range of interactions). Moreover, some general conclusions will be obtained for electrons in a periodical potential of a crystal.

The so-called correlation effects [8] between electrons are neglected here.

The principal assumption enabling us to obtain analytical results is:

$$\xi_k = \text{const}, \qquad \eta_k = \text{const}. \tag{18}$$

4. *Electrons with delta function interactions*

In this case $u_k(\boldsymbol{r}) = \text{const}$. Interaction energy is introduced in the form

$$G(|\boldsymbol{r}-\boldsymbol{r}'|) = V'\delta(\boldsymbol{r}-\boldsymbol{r}'). \tag{19}$$

The total energy is equal to

$$E = E(\xi_k, \varphi_k) = \sum_k \frac{\hbar^2}{2m}\left[k^2+k_z\xi_k\frac{1}{2\Delta}\int_0^{2\Delta}\frac{d\varphi_k}{dz}\,dz+\frac{1}{4}\frac{1}{2\Delta}\int_0^{2\Delta}\left(\frac{d\varphi_k}{dz}\right)^2 dz\right] +$$

$$+\frac{1}{2}\sum_{k,k'}V-\frac{V}{2}\sum_{k,k'}\left[1-\frac{(\varphi_k-\varphi_{k'})^2}{4}-\frac{(\xi_k-\xi_{k'})^2}{4}\right]+\sum_k\frac{\Omega}{N}K\frac{1}{2\Delta}\int_0^{2\Delta}\sin^2\varphi_k dz, \tag{20}$$

where $V = V'/\Omega$, $\Omega = L_xL_y2\Delta$ is the period volume, 2Δ is the width of two antiparallelly magnetized domains. We minimalize the energy (20) with respect to ξ_k, $\varphi_k(z)$ with the additional condition

$$\sum_k \xi_k = 0, \tag{21}$$

which we obtain from the formula (10). Next, we find $\varphi = \varphi(z)$ from the formula (17).

Taking into account (21), minimalization of (20) with respect to ξ_k leads to

$$\frac{\hbar^2}{2m}k_z\frac{1}{2\Delta}\int_0^{2\Delta}\frac{d\varphi_k}{dz}\,dz+\frac{V}{2}\sum_{k'}(\xi_k-\xi_{k'})+\lambda = 0, \qquad \sum_k \xi_k = 0, \tag{22}$$

where λ is the Lagrange factor. Minimalization with respect to $\varphi_k(z)$ leads to the Euler-Lagrange equations of the form

$$-\frac{1}{2}\frac{\hbar^2}{2m}\frac{d^2\varphi_k}{dz^2}+\frac{V}{2}\sum_{k'}(\varphi_k-\varphi_{k'})+\frac{\Omega}{N}K\sin 2\varphi_k=0. \tag{23}$$

The set of equations (22), (23) can be solved separately due to the assumption (18). We have $\frac{d\varphi_k}{dz}=\frac{d\varphi}{dz}$. In this case the Fermi surface is a sphere so that $\sum_k k_z=0$; therefore $\lambda=0$ from (21). We obtain

$$\xi_k=-2\frac{\frac{\hbar^2}{2m}\pi k_z}{VN\Delta}. \tag{24}$$

Using (9) we can write the equations (23) in the form

$$-\frac{1}{2}\frac{\hbar^2}{2m}\frac{d^2\varphi}{dz^2}+\frac{V}{2}\sum_{k'}(\eta_k-\eta_{k'})+\frac{\Omega}{N}K\sin 2(\varphi+\eta_k)=0 \tag{25}$$

and from (17) we have

$$\sum_k \eta_k=0. \tag{26}$$

Writing $\sin 2(\varphi+\eta_k)$ as a power series of η_k, substituting it into the equation (25) and using (26), we have

$$-\frac{1}{2}\frac{\hbar^2}{2m}\frac{d^2\varphi}{dz^2}+\frac{\Omega}{N}K\left[1-\frac{2}{N}\sum_k\eta_k^2\right]\sin 2\varphi=0. \tag{27}$$

This equation gives $\varphi=\varphi(z,\eta_k)$. We can see thus, that the exchange energy influences the distribution of φ through η_k only. The solution of the equation (27) with a periodical condition corresponding to the domains of the width Δ is [3]

$$\cos\varphi=-\operatorname{sn}\left[\frac{2\mathcal{K}}{\Delta}z-\mathcal{K}\right], \tag{28}$$

where

$$\mathcal{K}=\int_0^{\pi/2}\frac{d\beta}{\sqrt{1-\frac{K}{K+A\varepsilon^2}\sin^2\beta}}, \tag{29}$$

$$A=\frac{1}{4}\frac{\hbar^2}{2m}\frac{N}{\Omega}\frac{1}{1-\frac{2}{N}\sum_k\eta_k^2}, \qquad \varepsilon\to 0. \tag{30}$$

Substituting (28) into (27) and using the assumption that η_k are small we obtain after some

manipulations the set of equations for η_k. The solution not depending on z is

$$\eta_k = 0; \tag{31}$$

We find from (30) that

$$A = \frac{1}{4}\frac{\hbar^2}{2m}\frac{N}{\Omega}. \tag{32}$$

As a result of the minimalization procedure for this case we obtain the distribution of macroscopic magnetization directions in Bloch walls $\varphi = \varphi(z)$ given by (28), (29), (32) which has the same character as the magnetization distribution obtained in phenomenological theory [3] and in the Heisenberg model [5]. We can see that $\varphi_k = \varphi$ (because $\eta_k = 0$), *i.e.* projections of spins onto the XY plane lie along the macroscopical magnetization for all electrons; however, spins of different electrons deviate from the XY plane (the deviations are given by ξ_k), so they do not lie along the macroscopical magnetization! As a result, the macroscopical magnetization value in Bloch wall must be somewhat lower than that in the case of the ferromagnetic state with completely aligned spins. This result has been obtained earlier by means of the band model in the paper [10] and it is confirmed by experiments [11]. It may be expected in general that there may exist a state with a lower energy than that obtained in this paper. In such a state the assumption (18) would be not realized. Moreover, the value of macroscopical magnetization would not be constant in Bloch walls but it would be a continuous function of the variable z. This result has been obtained earlier by means of the Heisenberg model in papers [12] and [13]. In the paper [12] it was a result of spin wave excitations in domains and wall excitations in walls. In the paper [13] it was a result of lowering the value of exchange coupling between localised spins in Bloch walls caused by difference of directions of nearest neighbour spins. On the other hand, in our model the dependence of the macroscopical magnetization value on the position in walls is a result of deviations of electron quantization axes from the direction of magnetization even without the appearance of spin waves.

Using (28), we can obtain the Bloch wall width and the wall energy for the unit of wall surface. Defining the Bloch wall width δ by

$$\delta = \pi \left| \frac{d\varphi}{dz} \right|_{z_0}^{-1}, \tag{33}$$

where the subscript z_0 denotes that the derivative $\frac{d\varphi}{dz}$ is to be taken at the middle of the wall, we obtain

$$\delta = \pi \sqrt{\frac{\frac{1}{4}\frac{\hbar^2}{2m}\frac{N}{\Omega}}{K}}. \tag{34}$$

For $r_s = 2.5$ (where r_s is the mean radius of the volume corresponding to one electron in the Bohr units) and for $K \approx 10^6$ erg/cm^3 we obtain $\delta = 1.1 \cdot 10^{-5}$ cm. This result seems

to be plausible in comparison with the phenomenological theory and it indicates that the quantity A given by (32) plays the role of the "stiffness parameter".

The wall energy (for unit of wall surface) defined by

$$\sigma = \frac{E - E_0}{2L_x L_y} \tag{35}$$

is in the state with minimalized energy equal to

$$\sigma = 4\sqrt{\left(\frac{1}{4}\,\frac{\hbar^2}{2m}\,\frac{N}{\Omega}\right)K} - \frac{\pi^2\hbar^4}{20m^2}\,\frac{k_{\max}^2}{V'\Delta}, \tag{36}$$

where $k_{\max}$ denotes the wave vector at the Fermi level. The second term in the equation (36), originating from exchange energy and nonvanishing only if ξ_k are different from zero, shows that the total energy is actually reduced if electron spins can deviate from the XY plane in the proper way (24).

The formula (36) shows also that the ferromagnetic state is nonstable with respect to the spontaneous appearance of domain structure if the electron density becomes higher than the critical density for which both terms in (36) are equal. We would have some kind of a helical structure with a nonlinear distribution of magnetization directions!

5. *Electrons with Coulomb interactions*

In this case we proceed in a manner similar to that in the Section 4. The total energy is now equal to

$$E = \sum_{k} \frac{\hbar^2}{2m}\left[k^2 + k_z\xi_k\,\frac{1}{2\Delta}\int_0^{2\Delta}\frac{d\varphi_k}{dz}\,dz + \frac{1}{4}\,\frac{1}{2\Delta}\int_0^{2\Delta}\left(\frac{d\varphi_k}{dz}\right)^2 dz\right] +$$

$$+ \frac{1}{2}\sum_{k,\,k'}\left\langle kk'\left|\frac{e^2}{|r-r'|}\right|kk'\right\rangle - \frac{1}{2\Omega}\sum_{kk'}\frac{4\pi e^2}{|k-k'|^2}\left[1 - \frac{(\xi_k-\xi_{k'})^2}{4} - \frac{(\varphi_k-\varphi_{k'})^2}{4}\right] +$$

$$+ \sum_{k}\frac{\Omega}{N}K\,\frac{1}{2\Delta}\int_0^{2\Delta}\sin^2\varphi_k\,dz. \tag{37}$$

The minimalization in respect to ξ_k gives

$$\frac{\hbar^2}{m}\,k_z\,\frac{1}{2\Delta}\int_0^{2\Delta}\frac{d\varphi_k}{dz}\,dz + \frac{e^2}{\Omega}\sum_{k,\,k'}\frac{4\pi}{|k-k'|^2}\,(\xi_k-\xi_{k'}) + \lambda = 0, \qquad \sum_k \xi_k = 0. \tag{38}$$

We can solve the equations (38) by means of the procedure presented in the paper [6]. We introduce

$$\gamma = \frac{\hbar^2}{me^2}\,\frac{\pi}{\Delta} \tag{39}$$

and we can show that $\lambda = 0$ exactly as in the Section 4; equation (38) gives then

$$\gamma k_z + \frac{1}{\Omega} \sum_{k,k'} \frac{4\pi}{|k-k'|^2} (\xi_k - \xi_{k'}) = 0, \qquad \sum_k \xi_k = 0. \tag{40}$$

The solution is [6]

$$\xi(y) = \frac{y_z}{y} R(y), \tag{41}$$

where

$$R(y) = 4\pi\gamma \left[-\frac{243}{610} y - \frac{9}{122} y^3 \right], \tag{42}$$

$$y = k/k_{\max}. \tag{43}$$

The minimalization of (37) with respect to $\varphi_k(z)$ gives the Euler-Lagrange equation of the form

$$-\frac{1}{2} \frac{\hbar^2}{2m} \frac{d^2\varphi_k}{dz} + \frac{1}{2\Omega} \sum_{k'} \frac{4\pi e^2}{|k-k'|^2} (\varphi_k - \varphi_{k'}) + \frac{\Omega}{N} K \sin 2\varphi_k = 0. \tag{44}$$

The same procedure as in the Section 4 gives the solution (28), (29), and (34). For the wall energy (35) we obtain, however, another expression

$$\sigma = 4 \sqrt{\left(\frac{1}{4} \frac{\hbar^2}{2m} \frac{N}{\Omega} \right) K} - \frac{N}{\Omega} \frac{\hbar^4 \pi^2}{8m^2 e^2 \Delta} 0.7217\, \pi k_{\max}, \tag{45}$$

because the angles ξ_k are now given by (41), (42), (43) rather than by (24), as in the previous section.

In this case the ferromagnetic state becomes also unstable with respect to the spontaneous appearance of domain structure if the electron density is high enough. On the other hand, however, it is known [8] that the ferromagnetic state is unstable with respect to a paramagnetic state if this density is not low enough. It would be very interesting to verify whether both instability conditions are the same and which the state has a lower energy, or whether there exist stability regions for these three states. Unfortunately, no investigations of stability of the ferromagnetic state with respect to the paramagnetic one have been made up to now for the gas electrons in a crystal if anisotropic interactions between them are taken into account.

6. Electrons in a periodical potential of a crystal

A similar procedure can be applied in principle for electrons in a crystal if a periodical potential of a crystallographic lattice is taken into account. For example, in a nearly free electron approximation, it is possible to introduce

$$u_k(r) = 1 + b_k \sum_{l_0} e^{i l_0 r} \tag{46}$$

instead of $u_k(r) = \text{const}$, where l_0 are the vectors to nearest neighbours in a reciprocal lattice. The calculation of the total energy can be made on the same lines as in the previous

sections. However, the minimalizing procedure gives now a set of nonlinear equations which cannot be solved separately for ξ_k and $\varphi(z)$ even if only a very weak modulation of plane wave due to a periodical potential of a crystallographic lattice ($b_k \ll 1$) is taken into account. In this case one expects that the solution must be given by (28) with a small modulation from the lattice.

The situation of electrons in a crystal in a tight binding approximation is still more complicated. It is possible to consider one-band model with short range interactions different from zero only if electrons are in the same Wannier state. It is possible also to approximate Wannier states by atomic functions for calculations of total energy as in the previous sections. The minimalization procedure in this case gives a set of equations which can only be solved numerically.

7. *Conclusions*

We see that it is possible to obtain the distribution of magnetization directions in the Bloch walls and the wall width from the itinerant electron model of ferromagnetism if anisotropy energy is taken into account. In the most crude model, in which electrons in a crystal are treated as free electron gas, the solution is the same as in the phenomenological theory or in the Heisenberg model. In real crystals, this distribution must be modulated by a periodical potential of a crystallographic lattice.

We have found that the magnetization in Bloch walls must be a little lower than in domains or, more precisely, than in the strictly aligned ferromagnetic state. One can expect, that it is plausible in general to speak about local values of magnetization as a function of a position.

We have shown that the parameter A given roughly by (32) plays the role of the "stiffness parameter" of the phenomenological theory. It is an interesting fact that in our model this stiffness stems from kinetic electron energy, which "prevents" the change of the magnetization direction. One can expect, that if the problem is solved more strictly, some dependence of the angles ξ_k, η_k on z is possible, and that exchange interaction gives also some contribution to the stiffness in a similar way as in the papers [6] and [7].

We have found that in some conditions concerning electron density an instability of the ferromagnetic state with respect to the spontaneous appearance of assumed domain structure (or "helical structure") is to be expected. However, it is not certain whether instability with respect to the paramagnetic state is not more important. The elucidation of the last question requires further investigations.

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