SPIN WAVES IN BAND MODEL OF FERROMAGNETIC THIN FILMS

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Magnetic properties of ferromagnetic thin films in the band model are calculated in a manner analogous to that used for bulk bodies. The formula for spin wave energy spectrum is obtained with respect to the boundary conditions. The spontaneous magnetization is calculated starting from the free energy. Some properties of spin waves are discussed.

I. Introduction

Magnetic properties of ferromagnetic thin films have been investigated by means of the molecular field method at high temperatures [1, 2] and the spin wave theory in the Bloch [3–7] and Holstein-Primakoff [8, 9] formulation at low temperatures. The Green function method has been applied in [10, 11] and the band model has been adapted to the investigation of the thin film magnetism in [12].

The purpose of this paper is to present the spin wave theory of ferromagnetic thin films of metals from the point of view of the band model based on Valenta's model of the sublattices [1].

II. Model of a thin ferromagnetic film

Thin film is considered as a superposition of n monoatomic layers parallel with the surfaces of the film and with a certain crystallographic plane. The periodicity conditions are satisfied in the plane of a layer and the lack of a part of neighbours for the boundary layers is taken into account in the direction perpendicular to the surfaces. The position of an atom in a plane of the idealized crystallographic lattice is given by the two-dimensional vector $\boldsymbol{j}$, the layers are labelled by ν.

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We consider a simple model in which it is assumed that the intra-atomic exchange coupling of spins from two degenerate bands is responsible for the appearance of ferromagnetism. We take into account only the case when the Fourier transform of exchange integral does not depend on the wave vector [13, 14].

III. Electron energy eigenstates

To formulate and discuss the properties of ferromagnetic thin films in the band theory the effective mass approximation for the one electronic energy eigenvalues, very often applied in this problem [6, 13, 15, 16], can be used. Thus

$$E_{\tau \boldsymbol{h}} = \varepsilon_0[\boldsymbol{h}^2+(\pi(\tau-1)/n)^2] \tag{1}$$

where $\varepsilon_0 = \hbar^2/2m^*$ leaving out the energy of the ground state of the band.

The one electronic state $(\tau, \boldsymbol{h})$ belonging to the considered energy eigenvalues $E_{\tau \boldsymbol{h}}$ is determined as

$$|\tau \boldsymbol{h}, m> = c^+_{\tau \boldsymbol{h},m}|0> = \frac{1}{N}\sum_{\nu \boldsymbol{j}} \exp(-i\boldsymbol{h}\boldsymbol{j})\, \Gamma^{\boldsymbol{h}}_{\nu\sigma}\, c^+_{\nu \boldsymbol{j},m}|0> \tag{2}$$

by means of the creation and annihilation operators $c^{\pm}_{\tau \boldsymbol{h},m}$ in the Bloch representation and analogous operators $c^{\pm}_{\nu \boldsymbol{j},m}$ in the Wannier representation. Both the operators have oriented spin $m = \downarrow (\uparrow)$. The transformation coefficients $\Gamma^{\boldsymbol{h}}_{\nu\tau}$ in case of the energy spectrum (1) are found to be of the form (*e. g.* [16])

$$\Gamma^{\boldsymbol{h}}_{\nu\tau} = [(2-\delta_{1\tau})/n]^{1/2} \cos\left(\frac{(\pi(\tau-1)}{n}\left(\nu-\frac{1}{2}\right)\right). \tag{3}$$

The simplified energy spectrum (1) is usually accepted in theories of thin films [6, 7, 13, 15, 16]. From the point of view of results obtained from the Green's function method in the tight binding approximation [17] this spectrum is based on the assumption that the thin film has the simple cubic (100) structure and that the nearest neighbouring atoms are situated in the nearest layers only. Two overlap integrals A_m and B_m have the usual meaning of the matrix elements in Wannier representation. They are assumed of the same order of magnitude

($K_\uparrow = 1$; the parameter K_m is defined as $K_m = A_m/B_m$ [17].

The trace of the electron density matrix represents the total charge and determines the Fermi level E_F as a function of the film thickness. In case of the energy spectrum (1) the Fermi level is of the form

$$E_F = \varepsilon_0 \boldsymbol{h}_F^2 = \varepsilon_0\left[2\pi+\pi^2\left(\frac{1}{3}n^2-\frac{1}{2}n+\frac{1}{6}\right)n^{-2}\right]. \tag{4}$$

The Fermi level lowers with the decrease of the number of the layers.

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IV. Spin waves in band model

Let us choose the ground state of a ferromagnetic thin film as the state with all the spins oriented in the same direction. The elementary magnetic excitation depends on the fact that the electron in the point $(\tau, \boldsymbol{h})$ in the Bloch representation changes the spin direction appearing in the point $(\tau+\lambda, \boldsymbol{h}+\boldsymbol{q})$. The spin wave with the propagation vector $(\lambda, \boldsymbol{q})$ is determined by the superposition of the elementary excitations. It corresponds to the operator of the magnon creation

$$S^{+}_{\lambda \boldsymbol{q}} = \sum_{\tau \boldsymbol{h}} b(\tau \boldsymbol{h}, \lambda \boldsymbol{q})\, c^{+}_{\tau+\lambda, \boldsymbol{h}+\boldsymbol{q}\uparrow} c^{-}_{\tau \boldsymbol{h}\downarrow}$$

with the linear combination coefficients $b(\tau \boldsymbol{h}, \lambda \boldsymbol{q})$. As it is shown in [9], the state $S^{+}_{\lambda \boldsymbol{q}}|0>$ represents the spin waves propagating in crystal. Taking into consideration the transformation (2) we obtain

$$S^{+}_{\lambda \boldsymbol{q}}|0> = \frac{1}{N^2} \sum_{\nu \boldsymbol{j}} e^{i\boldsymbol{q}\boldsymbol{j}} \sum_{\varrho \nu} T^{\boldsymbol{q}}_{\nu\lambda, \varrho \boldsymbol{r}} |\nu \boldsymbol{j}, \varrho \boldsymbol{r}> \tag{5}$$

where $T^{\boldsymbol{q}}_{\nu\lambda, \varrho \boldsymbol{r}} = \sum_{\tau \boldsymbol{h}} b\,(\tau \boldsymbol{h}, \lambda \boldsymbol{q})\, \Gamma^{\boldsymbol{h}+\boldsymbol{q}}_{\nu+\varrho, \tau+\lambda} \Gamma^{\boldsymbol{h}}_{\nu\tau} \exp\,(i\boldsymbol{h}\boldsymbol{r})$. This means that in the band model an electron changing the spin direction changes the site appearing at the distance of not only the nearest but also of any other neighbours, while in Heisenberg model elementary excitations occur only in one definite position.

The character of the amplitudes of the nearest neighbour excitations is the same in both models with the accuracy to the phase factor and the normalization constant value due to the form of the coefficients $b(t\boldsymbol{h}, \lambda \boldsymbol{q})$. For bulk crystals the phase shift is the same for both the models.

V. Contribution to spin wave resonances

In case of the general form of $b(\tau \boldsymbol{h}, \lambda \boldsymbol{q})$ some properties of the amplitudes $T^{\boldsymbol{q}}_{\nu\lambda, \varrho \boldsymbol{r}}$ can be studied in connection with the resonance effect in ferromagnetic thin films excited by a homogeneous external magnetic rf field b_x. The appearance of the internal effective magnetic field leads to the asymmetry of the boundary conditions for the electronic potential on the surfaces of the film with respect to the orientation of the spin. The parameter determining these boundary effects for the spin *up* defined by the ratio of overlap integrals [17] is different than that for the spin *down*.

We consider three cases:

1. the asymmetry of the boundary conditions does not occur,
2. the difference p between the boundary parameters is very small $K_{\uparrow} = 1$, $(K_{\downarrow} = 1 + p)$,
3. large internal magnetic field acting in the opposite directions on the spins up and down respectively is assumed.

Starting from the formula for the probability for a transition from the ground state $|0>$ to the excited state $S^{+}_{\lambda \boldsymbol{q}}|0>$ defined by

$$P^{\lambda \boldsymbol{q}}_{0 \to 1} \sim |\sum_{\nu \boldsymbol{j}} b_x < 0 \,|\, S^{-}_{\lambda \boldsymbol{q}} c^{+}_{\boldsymbol{j}\uparrow} c^{-}_{\nu \boldsymbol{j}\downarrow} |0> |^2 \delta(\omega(\lambda \boldsymbol{q}) - \omega_{\mathrm{rez}})$$

and taking into consideration the representation for spin waves in the form given by (5) we can write the resonance condition in the form

$$\sum_{\nu j} \exp(i\boldsymbol{q}\boldsymbol{j}) \left[\sum_{\nu\hbar} b(\tau\hbar, \lambda\boldsymbol{q})\ \Gamma^{\hbar+\boldsymbol{q}}_{\nu,\tau+\lambda}\tilde{\Gamma}^{\hbar}_{\nu\tau}\right] \neq 0 \tag{6}$$

in which the solution $\tilde{\Gamma}^{\hbar}_{\nu\tau}$ is a consequence of the above mentioned assumptions. If the formula (3) represents the solution for the spin up, $\tilde{\Gamma}^{\hbar}_{\nu\tau}$ for the spin down are of the form:

1. given by formula (3)

2. $$\tilde{\Gamma}^{\hbar}_{\nu\tau} = [(2-\delta_{1\tau})/n]^{1/2} \cos\left[(\pi(\tau-1)+\beta)\left(\nu-\frac{1}{2}\right)\Big/ n-\frac{1}{2}\beta\right] \tag{3a}$$

where

$$\beta = (n^2\mathrm{tg}^2[\pi(\tau-1)/n]+2np)^{1/2}-n\ \mathrm{tg}[\pi(\tau-1)/n]$$

3. $$\tilde{\Gamma}^{\hbar}_{\nu\tau} = [2/(n-1)]^{1/2} \sin[\pi(\tau-1)(\nu-1)/(n-1)] \quad \text{for} \quad \tau\in(2, n-1) \tag{3b}$$

and

$$\tilde{\Gamma}^{\hbar}_{\nu(\frac{1}{n})} = (1/\sqrt{2})(\delta_{1\nu}\pm\delta_{n\nu}).$$

It can be seen from the formula (6) that the resonance peaks appear for $\boldsymbol{q}=0$ onlyt which is in agreement with the experimental data. Taking into account the fact, that the $b(\tau\hbar, \lambda\boldsymbol{q})$ do not depend on the ν's, we find in considered cases:

1. The resonance peaks appear for $\lambda = 0$ only, which is in agreement with the resul obtained from Heisenberg model without the additional assumptions concerning the surface anisotropy field [9].

2. The sequence of the resonance peaks appears for even λ, which corresponds to the result obtained from the ferromagnetic resonance theory in Heisenberg model for very small pinning [18].

3. In this case the summation over ν is especially simple for sufficiently large number of layers n, *i. e.* in the most interesting region for experimental measurements, and it leads to the appearance of resonance peaks for odd λ and $\lambda = 0$ according to the results of the classical experiment [19] in this field of research. This picture corresponds to the large surface anisotropy field or to the case when the surface spins are completely pinned in Heisenberg model.

The power absorbed in the spin wave models per mode is inversely proportional to λ^2, which is the same result as that in Heisenberg theory.

Concluding we would like to notice that our results concerning the resonance effect obtained in the band model are equivalent to those from Heisenberg theory under the same assumptions from the physical point of view. However, the origin of the surface effects could be explained by means of the internal field. Thus the effect of the surface anisotropy field can be obtained directly from the boundary conditions concerning the lack of a part of neighbours for atoms in the boundary layers.

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VI. Spin wave energy spectrum

The energy of the excited state is expressed by means of interaction between the spin operators in the usual manner well known from the band model [13]. The spin wave dispersion relation for the above ferromagnetic model can be derived in a number of ways. The variational method and the random phase approximation seem to be the most convenient ones [13, 20, 21]. According to these procedures [13] adapted to the thin films we get the equation for the spin wave spectrum $\hbar\omega(\lambda\boldsymbol{q})$:

$$(I/N^2n)\sum_{\tau\boldsymbol{h}}[f(E_{\tau\boldsymbol{h}\uparrow})-f(E_{\tau\boldsymbol{h}\downarrow})]\,C(\tau\boldsymbol{h},\,\lambda\boldsymbol{q})=\pm 1 \tag{7}$$

where

$$C(\tau\boldsymbol{h},\,\lambda\boldsymbol{q})=[I\langle r\rangle-\hbar\omega(\lambda\boldsymbol{q})+E_{\tau+\lambda,\,\boldsymbol{h}+\boldsymbol{q}}-E_{\tau\boldsymbol{h}}]^{-1}$$

with the intra-atomic exchange integral I. $f(E)$ denotes the Fermi distribution function and $\langle r\rangle$ is the relative spontaneous magnetization of a thin film.

The coefficients $b(\tau\boldsymbol{h},\,\lambda\boldsymbol{q})$ are given by

$$b(\tau\boldsymbol{h},\,\lambda\boldsymbol{q})=\Delta^{-1}(\lambda\boldsymbol{q})\,C(\tau\boldsymbol{h},\,\lambda\boldsymbol{q}) \tag{8}$$

with the normalization condition

$$\Delta^2(\lambda\boldsymbol{q})=\sum_{\tau\boldsymbol{h}}[f(E_{\tau\boldsymbol{h}\uparrow})\,(1-f(E_{\tau\boldsymbol{h}\downarrow}))]\,C^2(\tau\boldsymbol{h},\,\lambda\boldsymbol{q}).$$

In the formula (7) the upper sign corresponds to the solution for the acoustic branch and the lower sign corresponds to that for the optical magnon spectrum. For $T=0$, $q=0$, $\lambda=0$ the optical magnon mode starts at $2I$ and the acoustic spin wave energy starts at $\hbar\omega(\lambda\boldsymbol{q})=0$ similarly to the case of bulk bodies.

To calculate the acoustic spin wave energy $\hbar\omega(\lambda\boldsymbol{q})$ analytically, for easy discussion of the results, we adapt the effective mass approximation. Elementary calculations lead to the following expression for the energy of magnons

$$\hbar\omega(\lambda\boldsymbol{q})=\varepsilon_0(D_1q^2+D_2(\pi\lambda/n)^2) \tag{9}$$

where

$$D_1=1-\frac{1}{\theta}\,\frac{D(1,2,h_F)-D(1,2,h_\theta)-2\bar{\theta}D(1,1,h_\theta)}{D(1,1,h_F)-D(1,1,h_\theta)} \tag{9a}$$

and

$$D_2=1-\frac{2}{\theta}\,\frac{D(2,2,h_F)-(D(2,2,h_\theta)-2\bar{\theta}D(2,1,h_\theta)}{D(1,1,h_F)-D(1,1,h_\theta)}. \tag{9b}$$

The introduced coefficients have the following meanings:

$$D(2,1,h)=(\pi^2/6n^3)x(2x^2-3x+1)$$

$$D(1,1,h)=(xh^2/n)-D(2,1,h)$$

$$D(2, 2, h) = 2D(2, 1, h)\,[h^2-(\pi^2/5n^2)\,(3x^2-3x-1)]$$

$$D(1, 2, h) = h^2\,D(1, 1, h)-\tfrac{1}{2}\,D(2, 2, h)$$

$$D(l, k, ih) = 0$$

$$h_\theta = (h_F^2-\theta)^{1/2};\ \theta = \theta - I/\varepsilon_0;\quad x = E\left(1+\frac{hn}{\pi}\right) \leqslant n.$$

It can be seen from the formula (9a) and (9b) that the energy spectrum depends on the number of the layers n. It shows also a slight anisotropy in the behaviour of the spectrum in the plane of the layer and that in the direction perpendicular to the film. For thick films htsi anisotropy vanishes and the values of both the coefficients D_1 and D_2 pass into the known value for the bulk bodies [13].

Comparing our results with the spin wave energy formula for Heisenberg model (6) it can be seen that the behaviour of the D_1 and D_2 corresponds to that of the effective exchange integral.

VII. Spontaneous magnetization

To discuss the spontaneous magnetization we must introduce the external magnetic field B into the energy of the excited states. As result we obtain the magnon energy spectrum given by

$$\hbar\bar{\omega}(\lambda\boldsymbol{q}) = 2\beta(B+B_r)+\hbar\omega(\lambda\boldsymbol{q})$$

where β is the product of the Bohr's magneton and the gyromagnetic factor and $\hbar\omega(\lambda\boldsymbol{q})$ is given by (9) in which I is replaced by $I+2\beta(B+B_r)$ in θ. The definition of $\bar{\theta}$ remains as before. The B_r denotes the internal effective magnetic field.

The calculation of the spontaneous magnetization by means of the thermodynamic function of free energy leads to the result

$$\langle r\rangle = 1 - \frac{1}{\sqrt{2\pi}}\,\frac{kT}{\varepsilon_0 D_1}\,\frac{1}{n}\sum_{\lambda=0}^{n-1}\ln\,[1-\exp\,(\gamma-\eta_\lambda)]^{-1} \tag{10}$$

where

$$\gamma = 2\beta\,B_r/kT;\ \eta_\lambda = (\pi^2\,\varepsilon_0\,D_2/kT)\,(\lambda/n)^2.$$

The result (10) is valid at low temperatures for films with $I > \varepsilon_0\,h_F^2$. The formula (10) determining the spontaneous magnetization as a function of the temperature and of the film thickness is analogous to that obtained in Heisenberg spin wave model [6] at low temperatures. Instead of Heisenberg exchange integral there exist the parameters D_1 and D_2 changing according to the change of the thickness.

In case of sufficiently large films and $I \ll \varepsilon_0\,h_F^2$ the magnon energy spectrum $\hbar\omega(\lambda\boldsymbol{q})$ in presence of an external magnetic field reduces to the result obtained by Morkowski [22] for bulk bodies. Thus one might expect, according to Morkowski's considerations, that the magnetization picture for $I \ll \varepsilon_0\,h_F^2$ will be changed; especially for temperatures near the Curie temperature.

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