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SURFACE POLARON IN SEMI-INFINITE FERROMAGNETIC SEMICONDUCTORS

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Within the framework of the exchange s-d model an excitation of surface and bulk waves in the semi-infinite cubic ferromagnetic semiconductors with surface (001) is investigated. By the method of two-time Green functions the dispersion relation for spin waves is derived. At different values of the overlap (hopping) integral parameter L the relation obtained is applied to wide-band and narrow-band ferromagnetic semiconductors. In the case $L \gg I$ (I – parameter of contact integral) this relation allows one to discuss the behavior of the surface and bulk spin waves in the ferromagnetic isolators.

The s-d model has been used to describe the excitations in the semi-infinite ferromagnetic semiconductor, by many authors. In these papers calculations were carried out by the method of two-time Green's functions. The semi-infinite magnetic semiconductor is the least studied case among semi-limited magnetic crystals. In the calculation of the surface excitations for conducting magnetic media the additional equations due to the presence of the conduction electrons appear, which form a system of equations for localized spins. The solving of such system in a general case causes considerable difficulties and it is necessary to find an approximate approach in order to overcome these difficulties. In paper [1] the magnetic excitations in the semi-infinite antiferromagnetic and ferrimagnetic semiconductors were studied at low temperatures without considering the overlap (hopping) integral. In paper [2] under the same conditions the magnetic excitations were considered in the semi-infinite ferromagnetic semiconductors. Taking into consideration the overlap (hopping) integral as a small parameter, the authors of the paper [3] calculated the spectrum of the surface spin waves in the semi-infinite ferromagnetic semiconductors.

In our paper we also use an approximate approach to solve the system of additional equations in the case of nonzero overlap integral, i.e. for $L \neq 0$. In contrast with the paper [3], our approach leads to the expression of the Green's function pole, which includes the energy dependent

ratio of the type $\frac{\varphi(E)}{\tan \varphi(E)}$. There are certain (critical) values of the angle $\varphi(E)$, which satisfy the condition

$\frac{\varphi(E)}{\tan \varphi(E)} = 1$. For these values of the angle $\varphi(E)$, we

examine the elementary excitations in the semi-infinite ferromagnetic semiconductors

The Hamiltonian of the semi-infinite ferromagnetic semiconductor, describing the s - d (or f - d) interaction model, has the following form [2]:

$$H = \sum_{j,\Delta,\sigma} L_{j,j+\Delta} a_{j\sigma}^+ a_{j+\Delta,\sigma} - \frac{1}{2} \sum_{j,\Delta} J_{j,j+\Delta} S_j S_{j+\Delta} - g\mu_B H_0 \sum_j S_j^z - g_e \mu_B H_0 \sum_j s_j^z - I \sum_j \{ S_j^z (a_{j\uparrow}^+ a_{j\uparrow} - a_{j\downarrow}^+ a_{j\downarrow}) + S_j^+ a_{j\downarrow}^+ a_{j\uparrow} + S_j^- a_{j\uparrow}^+ a_{j\downarrow} \}, \quad (1)$$

where $J_{j,j+\Delta}$ and $L_{j,j+\Delta}$ are exchange and overlap (hopping) integrals for the nearest neighbors of localized and non-localized spins, respectively, H_0 is the constant magnetic field directed along the axis Oz , I is the contact integral. To investigate magnetic excitations in the examined system, we introduce the two-time temperature dependent retarded Green's function as follows [2]:

$$G_{j,j'}(t-t') = \langle\langle S_j^+(t); S_{j'}^-(t') \rangle\rangle, \\
H_{j,j'}(t-t') = \langle\langle a_{j\uparrow}^+(t) a_{j\downarrow}(t) S_{j'}^-(t') \rangle\rangle, \quad (2)$$

For the Green's functions in (2) we use the following Fourier transform with respect to both time and the xy plane :

$$G_{j,j'}(t-t') = \frac{1}{N_s} \sum_{q_{\parallel}} \frac{1}{2\pi} \int dE e^{-iE(t-t') + iq_{\parallel}(r_j - r_{j'})} G_{j_{\perp}; j'_{\perp}}(E; \mathbf{q}_{\parallel})$$

$$H_{j,j'}(t-t') = \frac{1}{N_s^{3/2}} \sum_{k_{\parallel}, k'_{\parallel}, q_{\parallel}} \frac{1}{2\pi} \int dE e^{-iE(t-t') + i(k_{\parallel} - k'_{\parallel})r_j - iq_{\parallel}r_{j'}} H_{j_{\perp}; j'_{\perp}}(E, \mathbf{k}_{\parallel}, \mathbf{q}_{\parallel}) \quad (3)$$

where N_s is the number of sites at the layer, j_{\perp}, j'_{\perp} are the layers numbers, $\mathbf{k}_{\parallel} = (k_x, k_y)$ and $\mathbf{q}_{\parallel} = (q_x, q_y)$ are two-dimensional wave vectors for a conduction electron and a magnon, respectively. There exists a simple connection between these two vectors: $\mathbf{k}_{\parallel} - \mathbf{k}'_{\parallel} = \mathbf{q}_{\parallel}$. Since surface excitations are characterized by the two-dimensional wave vector parallel to the surface and by the damping parameter, which describes the excitation amplitude as a function of the distance from the surface, the solution of the system of equations for the Green's functions in (2) may be taken in the following form (at fixed j'_{\perp}):

$$G_{j_{\perp}; j'_{\perp}}(E; \mathbf{q}_{\parallel}) = A(E; \mathbf{q}_{\parallel}) e^{-\mu j_{\perp}}, \quad (4)$$

$$H_{j_{\perp}; j'_{\perp}}(E; \mathbf{k}_{\parallel}, \mathbf{q}_{\parallel}) = B(E; \mathbf{k}_{\parallel}, \mathbf{q}_{\parallel}) e^{-\mu_1 j_{\perp} - \mu_2 j'_{\perp}},$$

Substituting the expression (4) into equations for the Green functions in (2), we obtain the equation chain for each equations in (2). Each equation from that and another chains form in pairs the closed system for coefficients $A(E; \mathbf{q}_{\parallel})$ and $B(E; \mathbf{k}_{\parallel}, \mathbf{q}_{\parallel})$, respectively. Excluding the unknown $B(E; \mathbf{k}_{\parallel}, \mathbf{q}_{\parallel})$ from the each closed system, it is possible to obtain the equation chain with respect to $e^{-j_{\perp}\mu} A(E; \mathbf{q}_{\parallel})$ ($j_{\perp} = 0, 1, 2, 3, \dots$):

$$\left\{ \begin{aligned} & E - 2\sigma_s^s I_s - g\mu_B H_0 - S(J_s(0) - J_s(\mathbf{q}_{\parallel})) - SJ(1 - e^{-\mu}) - \\ & - \sum_{k_{\parallel}} \frac{4S\sigma_s^s (I_s)^2}{E - 2SI_s - L_s(k_{\parallel}) + L_s(k_{\parallel} + q_{\parallel}) - g_e \mu_B H_0 - L_s(e^{-\mu_2} - e^{\mu_1})} \end{aligned} \right\} A(E; \mathbf{q}_{\parallel}) = \frac{S}{\pi} \delta_{0, j_{\perp}} \quad j_{\perp} = 0$$

$$\left\{ \begin{aligned} & E - 2SI - g\mu_B H_0 - S(J(0) - J(\mathbf{q}_{\parallel})) - 2SJ(1 - \cosh \mu) \\ & - \sum_{k_{\parallel}} \frac{4S\sigma^s (I)^2}{E - 2SI - L(k_{\parallel}) + L(k_{\parallel} + q_{\parallel}) - g_e \mu_B H_0 - 2L(\cosh \mu_2 - \cosh \mu_1)} \end{aligned} \right\} e^{-\mu} A(E; \mathbf{q}_{\parallel}) = \frac{S}{\pi} \delta_{1, j_{\perp}}, \quad j_{\perp} = 1$$

$$\left\{ \begin{aligned} & E - 2SI - g\mu_B H_0 - S(J(0) - J(\mathbf{q}_{\parallel})) - 2SJ(1 - \cosh \mu) \\ & - \sum_{k_{\parallel}} \frac{4S\sigma^s (I)^2}{E - 2SI - g_e \mu_B H_0 - L(k_{\parallel}) + L(k_{\parallel} + q_{\parallel}) - 2L(\cosh \mu_2 - \cosh \mu_1)} \end{aligned} \right\} e^{-2\mu} A(E; \mathbf{q}_{\parallel}) = \frac{S}{\pi} \delta_{2, j_{\perp}}, \quad j_{\perp} = 2 \quad (5)$$

and etc.,

where

$$J_s(0) = 4J_s; J_s(\mathbf{q}_{\parallel}) = 2J_s(\cos aq_x + \cos aq_y)$$

$$L_s(k_{\parallel}) = 2L_s(\cos aq_x + \cos aq_y); L_s(\mathbf{k}_{\parallel} + \mathbf{q}_{\parallel}) = 2L_s(\cos a(k_x + q_x) + \cos a(k_y + q_y)).$$

The last expressions are valid also for $J(0)$, $J(\mathbf{q}_{\parallel})$, $L(\mathbf{k}_{\parallel})$ and $L(\mathbf{k}_{\parallel} + \mathbf{q}_{\parallel})$, but without the subscript s , which is the index of the free surface. For simplicity we have introduced in (5) the following notations for the exchange, overlap (hopping) and contact integrals: J_s , L_s and I_s , on the surface and J , L and I inside the crystal. We also denote the z component of the mean spin deviation of the conduction electron on the surface as $\sigma_s^s = \langle s_s^z \rangle$ and inside the crystal as $\sigma^s = \langle s^z \rangle$, respectively.

This system of equations in (5) coincides with the equation (3b) in paper [3]. In both cases, the spectrum of elementary excitations is determined by poles of Green's functions of localized spins. Depending on the value of the damping parameter μ we have spin waves either for bulk ($|e^{\mu}| = 1$) or for surface ($|e^{\mu}| < 1$). Because of the sum over the two-dimensional wave vectors of conduction

electrons in (5) the spectrum determination experiences difficulties. In order to overcome these difficulties we apply an approximate approach, which consists of the replacement of the sum over the wave vector \mathbf{k}_{\parallel} by the integral. Furthermore, passing in the system (5) from the sum to the corresponding integral over the wave vector \mathbf{k}_{\parallel} , it is possible to calculate the contribution of conduction electrons to the spectrum of the surface spin waves. The integral should be taken over all allowed values of the wave vector in the first Brillion zone. Expressions, obtained after the integration, by the trigonometrically transformations [4], are taken through the ratio of some angle depending on the energy to its tangent $\frac{\varphi(E)}{\tan \varphi(E)}$.

Thus, the Green's function pole for localized spins is given by the following equation:

$$E - 2 \sigma^S I - g \mu_B H_0 - 4JS(1 - \cos aq_x) - 2JS(1 - \cosh \mu) + \frac{2S\sigma^S(I)^2}{\pi L \sin aq_x} \frac{\varphi(E)}{\tan \varphi(E)} = 0, \quad (6)$$

where

$$e^{\mu} = 1 + 2 \frac{I}{J} \left(1 - \frac{I_s \sigma^S}{I \sigma^S} \right) \frac{\sigma^S}{S} + 4 \left(1 - \frac{J_s}{J} \right) (1 - \cos aq_x) + \frac{2\sigma^S(I/J)^2}{\pi(L/J) \sin aq_x} \left(\frac{\varphi(E)}{\tan \varphi(E)} - \frac{(I_s/I)^2 \sigma^S}{(L_s/L) \sigma^S} \frac{\varphi_0(E)}{\tan \varphi_0(E)} \right)$$

$$\varphi_0(E) = \arctan \frac{\sqrt{\lambda_0^2 - 1}}{\cos(\frac{1}{2} aq_x)} \quad \varphi(E) = \arctan \frac{\sqrt{\lambda^2 - 1}}{\cos(\frac{1}{2} aq_x)}$$

$$\lambda_0 = \frac{2SI_s + g_e \mu_B H_0 + L_s e^{\mu} - E}{4L_s \sin(\frac{1}{2} aq_x)}$$

$$\lambda = \frac{2SI + g_e \mu_B H_0 + 2L(\cosh \mu_2 - \cosh \mu_1) - E}{4L \sin(\frac{1}{2} aq_x)}$$

Though the integration leads the system (5) to more simple form as in (6), the functional dependence $\varphi(E)$ complicates its solution both analytically and graphically. Therefore, the problem to solve this equation even at some values of the angle $\varphi(E)$ occurs. For simplicity such values $\varphi(E)$, at which the condition $\frac{\varphi(E)}{\tan \varphi(E)} = 1$ is

fulfilled, are used for the calculation of the spectrum. Consequently, these values of the angle $\varphi(E)$ are determined from the solution of the (graphical) equation [5]:

$$\tan \varphi_i(E) = \varphi_i(E) \quad (i=0, 1, 2, \dots) \quad (7)$$

At the result the following values: $0; 1.43\pi; 2.46\pi; 3.47\pi$; for the angle $\varphi(E)$ were obtained. It should be noted, that the certain energy band corresponding to each of these values of the angle $\varphi(E)$, just as levels of free atoms with the energy ε_i are dissolved in energy bands in the solid state.

Thus, our considerations show that equation (6) allows one to describe the magnetic excitations in both wide-band ($W \gg SI$) and narrow-band ($W \leq SI$) ferromagnetic semiconductors with surface (001).

The dependence of the energy spectrum on the wave vector is presented in fig. 1 and 2.

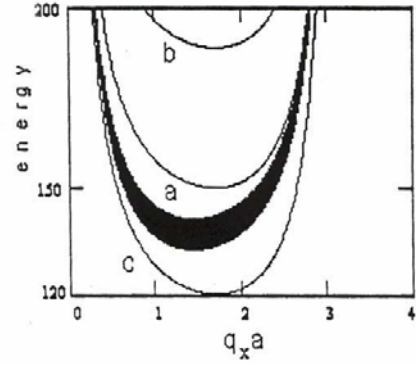


Fig. 1. The spin-wave frequencies plotted (in unit JS against $q_x a$ for a semi-infinite ferromagnetic semiconductors with $L \neq 0$. The parameter values are $g_e = g = 0.2$; $J_s = 0.5$ $\sigma^S = \langle s^Z \rangle = 0.5 = \sigma_s^S = \langle s_s^Z \rangle$; $S = \langle S^Z \rangle = 0.5$; $L = 55$; $L_s = 60$; and the labeling of the surface spin-wave branches corresponds to a , $I_s = 1.4$; b , $I_s = 1.6$; c , $I_s = 1.26$; $I = 50$. The bulk spin-waves appear as a continuum in this plot with the upper and lower edges corresponding to $\cosh \mu = \pm 1$.

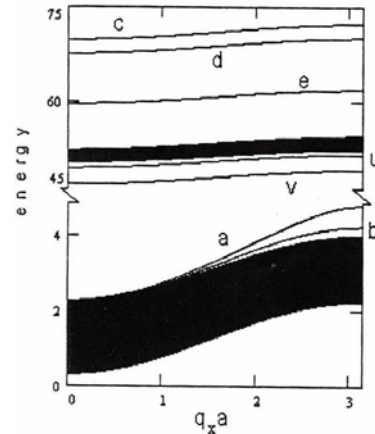


Fig. 2. Some numerical examples to illustrate the results for the spin-waves in the low frequency and high frequency excitations, respectively. The bulk spin-wave bands are shaded. The labeling of the surface spin-wave branches corresponds to $g_e = g = 0.3$; $J_s = 2$; $I = 50$; $\sigma^S = \langle s^Z \rangle = 0.5$ $\sigma_s^S = \langle s_s^Z \rangle = 0.5$; $S = \langle S^Z \rangle = 0.5$; a, c , $I_s = 20$; b, d , $I_s = 1.6$; e , $I_s = 40$; u , $I_s = 40$; v , $I_s = 54$

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