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ONE-PARTICLE EXCITATIONS IN A FERROMAGNETIC SEMI-INFINITE SEMICONDUCTOR SUPERLATTICE

TANRIVERDIYEV V.A., TAGIYEV V.S., SEYID-RZAYEVA S.M.

*Institute of Physics of National Academy of Sciences of Azerbaijan
370143, Baku H.Javid ave. 33 E-mail: solstphs@physics.ab.az*

One-particle excitations in a ferromagnetic semiconductor semi-infinite superlattice are investigated by Green function method. Bulk like excitation frequencies in the random-phase-approximation is derived. The result are illustrated numerically

Recently, there has been a growing interest in superlattice (SL) which elementary unit consisting of different magnetic materials. The study of SL has been motivated by the idea that the properties of SL can be significantly different from those of their component materials. Many theoretical investigations on the magnetic SL have been carried out with different models and methods [1-3]. The semi-infinite ferromagnetic semiconductors are intensively investigated in ref. [4,5]. The properties of the superlattice formed from ferromagnetic semiconductor materials comparatively fewer have been studied.

In this paper we consider one-particle excitations in a simple-cubic ferromagnetic semiconductor superlattice model in which the atomic planes of material 1 alternate with material 2. Each atomic plane is assumed to be the [001] planes. Such systems seem to provide a new type of material which does not exist naturally. The conduction electron magnetization, the electron polarization and total electron density for the SL under consideration in this paper are defined by Green function method at low temperature.

The Hamiltonian describing the conduction electron of the system is expressed as the following

$$H_E = \sum_{i,j,\sigma} t_{i,j} a_{i\sigma}^+ a_{j\sigma} - 0.5 \sum_{i,\sigma} (I_i S_i + g_e \mu_B H_0) \sigma a_{i\sigma}^+ a_{i\sigma},$$

$$H_I = -0.5 \sum_i I_i (S_i^+ s_i^- + S_i^- s_i^+). \quad (1)$$

Here S_i is spin operators for the localized spins at sites i , H_0 is a static magnetic field applied in the z direction.

Also $t_{i,j}$ is a hopping term and I_i is a contact interaction energy. The spin operators s_i of the conduction

electron at site i can be expressed as $s_i^+ = a_{i\uparrow}^+ a_{i\downarrow}$, $s_i^z = 0.5(a_{i\uparrow}^+ a_{i\uparrow} - a_{i\downarrow}^+ a_{i\downarrow})$, where $a_{i\sigma}^+$ and $a_{i\sigma}$ Fermi-creation and -annihilation operators for an electron at site i and having a spin index σ . The values $\sigma = \pm 1$ corresponds to up and down projections of the electron spin with respect to z .

In order to obtain the conduction-electron magnetization we must define the one-electron Green's function $g_{i,j\sigma}(t) = \langle\langle a_{i\sigma}(t) | a_{j\sigma}^+(0) \rangle\rangle$. The equation of motion for the Fourier transform of the Green's function $g_{i,j\sigma}(\omega)$ in the random-phase-approximation have the following form:

$$[\omega + 0.5\sigma(g_e \mu_B H_0 + I_i \langle S_i^z \rangle)] g_{i,j\sigma}(\omega) - \sum_{\delta} t_{i,i+\delta} g_{i+\delta,j\sigma}(\omega) = \delta_{ij}. \quad (2)$$

We use the translational invariance in the xy plane to define the Fourier transform

$$g_{i,j\sigma}(\omega) = \frac{1}{N} \sum_{k_{\parallel}} g_{m,m'\sigma}(\omega, k_{\parallel}) \exp[ik_{\parallel}(r_i - r_j)], \quad (3)$$

where $k_{\parallel} = (k_x, k_y)$ is a two-dimensional wave vector parallel to the surface, m and m' are positive integers labeling the lattice planes that contain sites i and j , respectively.

Assuming that m -th layer is of material 1 and $(m+1)$ -th layers of material 2, one obtains the following set of equations

$$\begin{cases} (\omega + A_1)g_{m,m'\sigma}(\omega, k_{\parallel}) - t[g_{m-1,m'\sigma}(\omega, k_{\parallel}) + g_{m+1,m'\sigma}(\omega, k_{\parallel})] = \delta_{m,m'} \\ (\omega + A_2)g_{m+1,m'\sigma}(\omega, k_{\parallel}) - t[g_{m,m'\sigma}(\omega, k_{\parallel}) + g_{m+2,m'\sigma}(\omega, k_{\parallel})] = \delta_{m+1,m'} \end{cases} \quad (4)$$

where

$$A_{1(2)} = 0.5\sigma(g_e\mu_B H_0 + I_{1(2)}\langle S_{1(2)}^z \rangle) - 4(1 - \gamma(k_{\parallel}))t_{1(2)}, \quad \gamma(k_{\parallel}) = 1 - 0.5(\cos k_x a + \cos k_y a).$$

The system is also periodic in the z direction, which lattice constant is $d=2a$. According to Bloch's theorem we introduce the following plane waves [3,6]

$$g_{m+2,m'\sigma}(\omega, k_{\parallel}) = g_{m,m'\sigma}(\omega, k_{\parallel}) \exp[ik_z d] \quad (5)$$

One-electron Green's function are obtained using equations (4) and (5):

$$g_{m,m\sigma}(\omega) = \sum_{j=1}^2 b_1(\omega_{j\sigma}) / (\omega - \omega_{j\sigma}), \quad (6)$$

$$g_{m+1,(m+1)\sigma}(\omega) = \sum_{j=1}^2 b_2(\omega_{j\sigma}) / (\omega - \omega_{j\sigma}),$$

$$b_{1(2)}(\omega_{j\sigma}) = (\omega_{j\sigma} + A_{2(1)}) / (\omega_{j\sigma} - \omega_{l\sigma}), \quad (j \neq l).$$

The poles of one-electron Green's function occur at energies

$$\omega_{1(2)\sigma} = 0.5[-A_1 - A_2 \pm \sqrt{(A_1 + A_2)^2 - 4A_1A_2 + 8t^2(1 + \cos k_z d)}]. \quad (7)$$

Surface conduction–electron magnetization are defined by the one-electron Green's function $g_{1,1\sigma}(\omega, k_{\parallel})$.

Assuming that the surface layer is of material r , ($r=1,2$) and the second layer is of material r' ($r' \neq r$, $r'=1,2$) one obtains the following set of equation in the matrix form

$$\begin{pmatrix} \omega + A_s & -t & 0 \\ -t & \omega + A_{r'} & -t \\ 0 & -t(1 + 1/x_{\sigma}) & \omega + A_r \end{pmatrix} \cdot \begin{pmatrix} g_{1,m'\sigma}(\omega, k_{\parallel}) \\ g_{2,m'\sigma}(\omega, k_{\parallel}) \\ g_{3,m'\sigma}(\omega, k_{\parallel}) \end{pmatrix} = \begin{pmatrix} \delta_{1,m'} \\ \delta_{2,m'} \\ \delta_{3,m'} \end{pmatrix} \quad (8)$$

One-electron Green's function for the surface layer is obtained by solving the equation (8):

$$g_{1,1\sigma}(\omega) = (x_{\sigma} + 1) / (\omega - \omega_{s\sigma}), \quad (9)$$

$$\omega_{s\sigma} = (A_r - A_s) / x_{\sigma} - A_s,$$

$$A_s = 0.5\sigma(g_e\mu_B H_0 + I_s \langle S_s^z \rangle) - 4t_s(1 - \gamma(k_{\parallel})),$$

$$x_{\sigma} = 0.5[(A_r - A_s)(A_{r'} - A_s) / t^2 - 1 \pm$$

$$\pm \sqrt{[(A_r - A_s)(A_{r'} - A_s) / t^2 - 1]^2 + 4(A_r - A_s)^2 / t^2}.$$

Using (7) and (8) one can obtain the expression of the number of conduction – electron in the spin– up and spin– down

$$n_{m(m+1)\sigma} = \sum_{j=1}^2 \sum_k b_{1(2)}(\omega_{j\sigma}) / [\exp(\omega_{j\sigma} / k_B T) + 1]$$

$$n_{s\sigma} = \sum_{j=1}^2 \sum_k (1 + x_{\sigma}) / [\exp(\omega_{j\sigma} / k_B T) + 1] \quad (10)$$

$$b_{1(2)}(\omega_{j\sigma}) = (\omega_{j\sigma} + A_{2(1)}) / (\omega_{j\sigma} - \omega_{j'\sigma}), \quad j \neq j'.$$

Knowing the number of conduction electrons conduction–electron magnetization ρ_v , the electron polarization r_v ($0 \leq r \leq 1$) and total electron density n_v are defined by [7]

$$\begin{aligned} \rho_v &= (n_{v\uparrow} - n_{v\downarrow}) / (2N), \\ r_v &= (n_{v\uparrow} - n_{v\downarrow}) / (n_{v\uparrow} + n_{v\downarrow}), \\ n_v &= n_{v\uparrow} + n_{v\downarrow}, \quad v = m, m + 1, s \end{aligned}$$

Some numerical calculations to illustrate the results are given in fig. 1 and fig. 2. Fig. 2 shows the one-particle excitation frequencies plotted with $k_z d$ for the superlattice, while fig.1 shows those plotted with $k_x a$ for the materials 1 and 2. All these figures correspond to $0 \leq k_x a \leq \pi$ and $0 \leq k_y a \leq \pi$. The analysis of the results shows that the width of the bulk like excitation regions in the ferromagnetic semiconductors superlattice is depended on transverse components of wave vectors, contact interaction and hopping interaction between constituents.

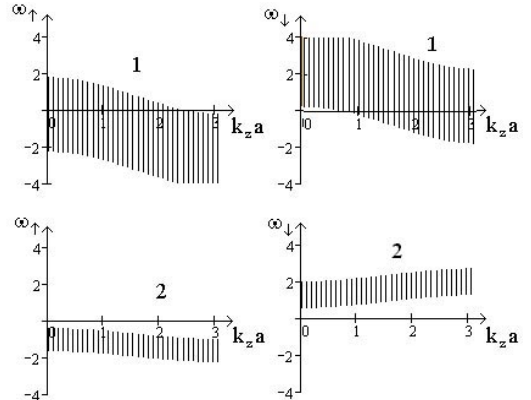


Fig.1. One-particle excitation frequencies plotted with $k_x a$ for the components 1 and 2. The parameters are $g_e\mu_B H_0 = 0.01 eV$, $I_1 = 2.5 eV$, $I_2 = 2.8 eV$, $t_1 = 0.5 eV$, $t_2 = 0.3 eV$, $S = 0.5$.

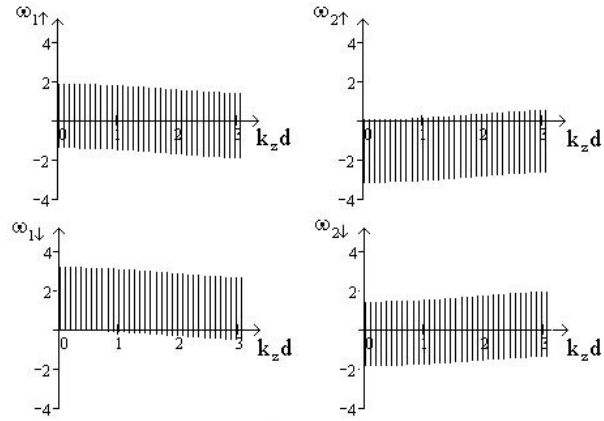


Fig.2. One-particle excitation frequencies plotted with $k_z d$ for the superlattice. The parameters are $g_e \mu_B H_0 = 0.01 \text{ eV}$, $I_1 = 2.5 \text{ eV}$, $I_2 = 2.8 \text{ eV}$, $t_1 = 0.5 \text{ eV}$, $t_2 = 0.3 \text{ eV}$, $t = 0.4 \text{ eV}$, $S = 0.5$.

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