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QUASI-TWO-DIMENSIONAL ELECTRON–HOLE LIQUID IN SHALLOW SiGe/Si QUANTUM WELLS

A. A. Vasilchenko,[1,2] G. F. Kopytov,[2] and V. S. Krivobok[3,4] UDC 538.915

An analytical expression is obtained for the energy of a quasi-two-dimensional electron-hole liquid (EHL) in shallow quantum wells. It is shown that in the $Si/Si_{1-x}Ge_x/Si$ *structures with small x, the EHL contains light and heavy holes. With increasing x, the transition of EHL to a state with heavy holes occurs, and the equilibrium density of electron-hole pairs strongly decreases. The effect of an external electric field on the EHL properties is studied.*

Keywords: electron-hole liquid, light and heavy holes, Schrödinger equation.

INTRODUCTION

Relatively recently, the possibility of the formation of a quasi-two-dimensional EHL in SiGe/Si quantum wells (QWs) has been demonstrated [1–6]. The spectrum of such an EHL is largely formed by the structure of the valence band, the density of states in which is nonmonotonic due to the presence of different hole subbands [6]. At the same time, according to the existing ideas, the appearance of jumps in the density of states should lead to the appearance of additional local minima in the dependence of the total energy of a two-component Fermi liquid on its concentration. Depending on which minimum is the main, the properties of the EHL will also change. As far as the authors are aware, there is no theoretical analysis of the effects of this type in the modern literature.

The available experimental results do indicate a modification of the EHL properties depending on the germanium composition in the SiGe layer. In particular, an unusual structure in the emission spectrum of the EHL in a SiGe/Si quantum well with small germanium composition (of several percent) was observed experimentally in [6]. The authors managed to explain the shape of the condensed phase line within the framework of the concepts on a multicomponent Fermi liquid containing both heavy and light holes. We note that the observed fine structure of the EHL emission spectra disappears with increasing germanium composition in the quantum well.

The aim of this paper is to find an analytical expression for the energy of a quasi-two-dimensional EHL with allowance for two types of holes. The theoretical approach in this study is similar to the one we used in [7]. To calculate the EHL energy, the density functional method is used.

THEORETICAL MODEL

In $Si/Si_{1-x}Ge_x/Si$ structures, a QW for holes and a barrier for electrons are formed in the SiGe layer. For small x, the values of the barrier height and well depth are small, and the effect of the barrier and well will not be

[1]Kuban State Technological University, Krasnodar, Russia, e-mail: a_vas2002@mail.ru; [2]Kuban State University, Krasnodar, Russia, e-mail: g137@mail.ru; [3]P. N. Lebedev Physical Institute, Moscow, Russia, e-mail: krivobok@sci.lebedev.ru; [4]National Research Nuclear University "MEPhI", Moscow, Russia. Translated from Izvestiya Vysshikh Uchebnykh Zavedenii, Fizika, No. 2, pp. 3–7, February, 2018. Original article submitted July 24, 2017.

taken into account in what follows. For an electrically neutral EHL with two types of holes, the total energy is written in the form

$$E_t[n_e,n_h]=T_e[n_e]+T_h[n_{hh}]+T[n_{hl}]+\int\Delta_{hl}n_{hl}(z)dz+E_{xc}\left[n_e,n_{hh},n_{hl}\right], \tag{1}$$

where T_e, T_{hh}, and T_{hl} are the kinetic energies of electrons, heavy, and light holes, respectively, E_{xc} is the exchange-correlation energy, Δ_{hl} is the splitting between the heavy and light holes, n_e , n_{hh}, and n_{hl} are the electron, heavy, and light hole densities, respectively.

Below, an exciton system of units is used, in which the energy is measured in units of $Ry_{ex} = e^2/2ka_{ex}$ and the length is measured in units $a_{ex}=k\hbar^2/\mu e^2$, where μ is the reduced mass and k is the dielectric permittivity.

Varying Eq. (1) with respect to the densities n_e , n_{hh}, and n_{hl}, we obtain three Schrödinger equations:

$$\left(-\frac{\mu}{m_{z,i}}\frac{d^2}{dz^2}+V_{xc,i}(z)\right)\psi_{n,i}(z)=E_{n,i}\psi_{n,i}(z), \tag{2}$$

where $i = e$, hh, and hl.

When only the lower level of the size quantization is filled, the carrier densities are given by the expressions

$$n_e(z)=N_e\psi_{0,e}^2(z),\ n_{hh}(z)=N_{hh}\psi_{0,hh}^2(z),\ n_{hl}(z)=N_{hl}\psi_{0,hl}^2(z), \tag{3}$$

where N_e, N_{hh}, and N_{hl} are the two-dimensional electron, heavy, and light hole densities, respectively. In what follows, the index “0” by variables will be omitted.

The kinetic energy can be written in the following form:

$$T_i[n_i]=\frac{\pi\mu}{g_i m_{d,i}}N_i^2+N_i(E_i-\int V_{xc,i}(z)\psi_i^2(z)dz), \tag{4}$$

where g_i is the number of equivalent valleys and $m_{d,i} = (m_{x,i}m_{y,i})^{1/2}$.

In Eq. (4), the first term corresponds to the total kinetic energy of carriers along the electron-hole layer, and the second term corresponds to the kinetic energy across the layer.

As in [7], we take $\varepsilon_{xc,i}=-0.91K/r_{s,i}$, where $r_{s,i}=(3/4\pi n_i)^{1/3}$ and K = 1.3. For each type of charge carriers, we use the local density approximation. Then, the exchange-correlation energy is written as

$$E_{xc,i}[n_i]=\int\varepsilon_{xc,i}n_i(z)dz\ . \tag{5}$$

For such a representation of energy, the exchange-correlation potential has the form

$$V_{xc,i}(z)=\frac{d(n_i\varepsilon_{xc})}{dn_i}. \tag{6}$$

To solve the Schrödinger equation, we use the approximate method proposed in [8]. For each type of charge carriers, we take the wave function with the parameter b_i in the form

$$\psi_i(z)=(1/(\pi^{1/2}b_i))^{1/2}\exp(-z^2/(2b_i^2))\ . \tag{7}$$

We expand $V_{xc,i}(z)$ in a series and, taking into account only the quadratic term in z, we obtain from the Schrödinger equation for each type of charge carriers that

$$b_i = (1.45\mu^{3/5} / (m_{z,i}^{3/5} K^{3/5} N_i^{1/5}), \tag{8}$$

$$E_e = -0.95 K^{6/5} N_e^{2/5} (m_{z,e} / \mu)^{1/5}, \tag{9}$$

$$E_{hh} = -0.95 K^{6/5} N_{hh}^{2/5} (m_{z,hh} / \mu)^{1/5}, \tag{10}$$

$$E_{hl} = -0.95 K^{6/5} N_{hl}^{2/5} (m_{z,hl} / \mu)^{1/5} + \Delta_{hl}. \tag{11}$$

Substituting the charge carrier densities in Eq. (1) and using Eqs. (3)–(11), we obtain the energy per one electron-hole pair:

$$E_{eh} = -0.69 K^{6/5} \left(\frac{m_{z,e}}{\mu}\right)^{1/5} N_e^{2/5} - 0.69 K^{6/5} \left(\frac{m_{z,hh}}{\mu}\right)^{1/5} \frac{N_{hh}^{7/5}}{N_e} - 0.69 K^{6/5} \left(\frac{m_{z,hl}}{\mu}\right)^{1/5} \frac{N_{hl}^{7/5}}{N_e}$$
$$+\pi \frac{\mu}{g_e m_{d,e}} N_e + \pi \frac{\mu}{m_{d,hh}} \frac{N_{hh}^2}{N_e} + \pi \frac{\mu}{m_{d,hl}} \frac{N_{hl}^2}{N_e} + \Delta_{hl} \frac{N_{hl}}{N_e}. \tag{12}$$

In Eq. (12), the first three terms correspond to the exchange and transverse kinetic energies of electrons, light, and heavy holes, respectively, the next three terms are the longitudinal kinetic energies of electrons, light, and heavy holes, respectively, and the last term is due to the splitting between heavy and light holes.

For an electrically neutral EHL, we have $N_e = N_{hh} + N_{hl}$. Taking into account that the Fermi energy of holes is $E_{\mathrm{F},i} = 2\pi\mu N_i / m_{d,i}$, we have

$$E_{hh} + \frac{2\pi\mu N_{hh}}{m_{d,hh}} = E_{hl} + \frac{2\pi\mu N_{hl}}{m_{d,hl}}. \tag{13}$$

From Eq. (13), we obtain

$$N_{hl} = N_e \frac{m_{d,hl}}{m_{d,hh} + m_{d,hl}} - \frac{m_{d,hh} m_{d,hl}}{m_{d,hh} + m_{d,hl}} \frac{E_{hl} - E_{hh}}{2\pi\mu}. \tag{14}$$

If we obtain $N_{hl} < 0$ from Eq. (14), then it is necessary to take $N_{hh} = N_e$ and $N_{hl} = 0$.

RESULTS

Calculations were carried out for the Si/SiGe/Si structure. For calculations, we used the following parameters [9, 10]: $\Delta_{hl} = 16.6x$, $g_e = 4$, $g_{hh} = g_{hl} = 1$, $m_{z,e} = 0.198m_0$, $m_{d,e} = 0.44m_0$, $m_{z,hh} = 0.28m_0$, $m_{d,hh} = 0.2m_0$, $m_{z,hl} = 0.18m_0$, and $m_{d,hl} = 0.25m_0$ (m_0 is the free electron mass).

First, we consider an EHL with one type of holes. From Eq. (12), we find the minimum energy, to which the equilibrium density of electron-hole pairs corresponds:

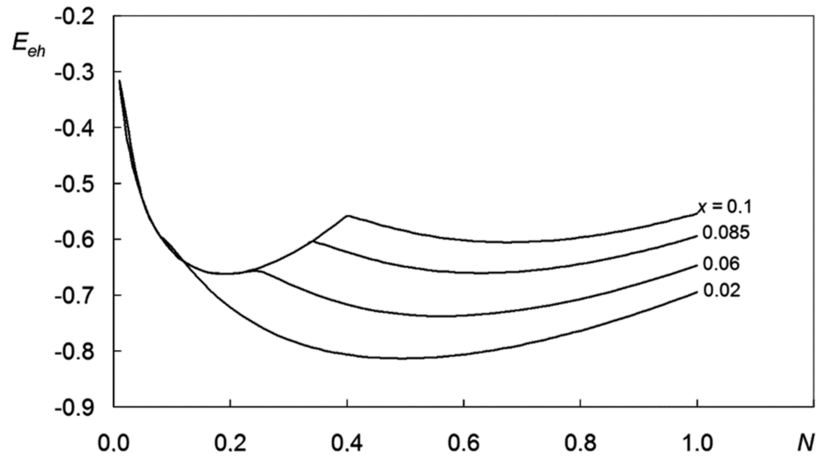

Fig. 1. Dependence of the energy per one electron-hole pair on the two-dimensional density of pairs.

$$N_{eh} = 0.037\mu^2 K^2 \frac{(m_{z,e}^{1/5} + m_{z,h}^{1/5})^{5/3}}{(1/g_e m_{d,e} + 1/m_{d,h})^{5/3}} . \tag{15}$$

It is seen from Eq. (15) that the equilibrium density depends relatively weakly on the transverse masses of charge carriers, whereas, it strongly depends on the number of valleys and longitudinal masses. Substituting the values of the parameters for SiGe, we obtain the equilibrium density N_{eh} = 0.21. Note that for $g_e m_{de} >> m_{dh}$, the equilibrium density will be proportional to $m_{dh}^{5/3}$ and in SiGe, the EHL with light holes will have an equilibrium density 1.5 times greater, than that in EHL with heavy holes.

Let us consider an EHL with two types of holes in the Si/SiGe/Si structure. It can be seen from Eqs. (10) and (11) that at close densities of light and heavy holes, it is possible to take into account only the splitting between heavy and light holes in the difference of the energy levels of holes: $E_{hl} - E_{hh} = \Delta_{hl}$.

Figure 1 shows the dependence of the energy per one electron-hole pair on the two-dimensional concentration of pairs N. At x = 0.02, the EHL contains two types of holes, and the energy minimum corresponds to N = 0.5. The calculated value of the equilibrium density is in good agreement with the experimental results [4, 6]. As x increases, two minima appear: the first minimum at smaller values of N corresponds to an EHL with heavy holes, and the second one corresponds to an EHL with light and heavy holes. At x = 0.085, the energy values in the first and second minima coincide, and as x increases, the main state of the EHL will be a state with heavy holes. We note that a similar transition was observed in the experiment [6].

As can be seen from Fig. 1, for small x, the equilibrium density of charge carriers is ~0.5 ($2\cdot10^{12}$ cm^{-2}), and in the state with heavy holes, the equilibrium density decreases approximately by a factor of three. In the range of values of x = 0.6–0.9, the energies of the two-component and one-component EHLs differ only weakly from each other. This means that bistability is possible in the system, at which a weak external effect can influence the properties of the EHL. Such external influence can be the pressure and the external magnetic or electric field. For example, by applying the compensating uniaxial pressure to the heterostructure, it is possible to change the splitting of hole states and thus, change the state of the EHL. The simplest way to influence the EHL is to apply an external electric field.

Let us consider in more detail the effect of an external electric field on the properties of an EHL. For a weak electric field, we can use the model proposed by us. Let the electric field be created by a gate with a surface charge N_t. In this case, the electroneutrality condition is written in the form $N_e + N_t = N_{hh} + N_{hl}$. To determine the density of light

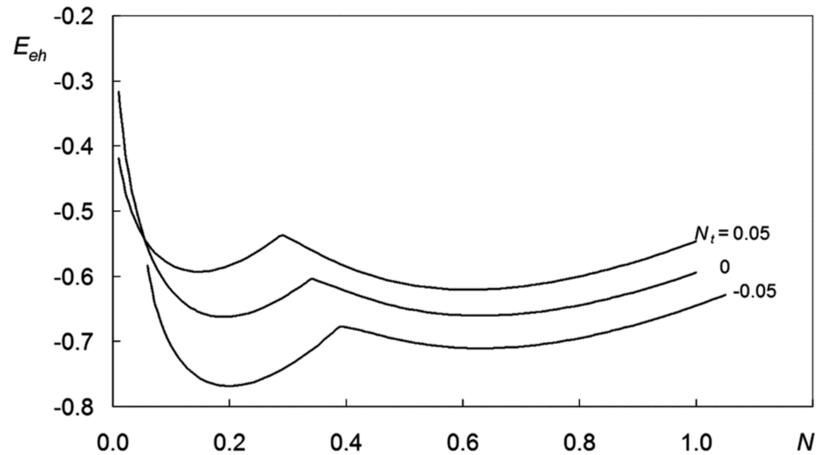

Fig. 2. Dependence of the energy per one electron-hole pair on the two-dimensional density of pairs (x = 0.085).

holes, it is necessary to use Eq. (14), replacing in it the value of N_e by $N_e + N_t$. In case of $N_t > 0$, the EHL will be positively charged and the energy per one electron-hole pair will be written as

$$E_{eh} = \frac{E_t(N_e, N_h) - E_t(0, N_t)}{N_e}, \tag{16}$$

where $E_t(N_e, N_h)$ is the total EHL energy and $N_h = N_{hh} + N_{hl}$.

For a negatively charged EHL, the energy per one electron-hole pair has the form

$$E_{eh} = \frac{E_t(N_e, N_h) - E_t(N_t, 0)}{N_h}. \tag{17}$$

The results of the calculations are shown in Fig. 2. We took the value of $x = 0.085$, at which the energy minima for an EHL with light and heavy holes and for that only with heavy holes are equal to each other. It is evident that at $N_t = 0.05$, the main state of the EHL will be a state with light and heavy holes. When the direction of the electric field changes, the EHL passes into a state with heavy holes. We note that for $N_t > 0$, the equilibrium density of electron-hole pairs decreases, and in case of negative N_t, it increases.

CONCLUSIONS

An analytical expression is obtained for the energy of a quasi-two-dimensional EHL in shallow quantum wells. The energy and equilibrium density of electron-hole pairs are calculated for the Si/SiGe/Si structure. It is shown that for small splitting between the energy levels of light and heavy holes, the EHL contains both light and heavy holes. As the splitting increases, a transition to an EHL with heavy holes takes place, and the equilibrium density decreases strongly. For the equilibrium density of electron-hole pairs, a satisfactory agreement has been obtained between the model and experimental results.

The effect of an external electric field on the properties of an EHL is studied. It is shown that in the EHL, bistability is possible, at which weak external impact can influence the properties of the EHL, and in case of a positively charged EHL, the minimum energy in the state with light and heavy holes decreases in comparison with the energy minimum of the EHL with heavy holes.

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