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Quasi-two-dimensional electron-hole liquid with two type of holes in SiGe/Si quantum wells

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Abstract. The density functional theory was used to calculate the energy of a quasi-two-dimensional electron-hole liquid (EHL) in Si/Si_{1-x}Ge_x/Si quantum wells. We have performed a numerical solution of the three one-dimensional nonlinear Schrödinger equations for electrons, heavy and light holes. It is shown that EHL contains heavy and light holes for small x . With an increase in x , a transition to a state with one type of hole occurs, and the density of electron-hole pairs decreases by more than three times. The results of the calculations are in good agreement with the experimental results.

1. Introduction

Investigation of the properties of electron-hole systems is one of the actively developing areas of modern condensed matter physics. At present, the greatest attention is paid to low-dimensional electron-hole systems, in which the role of the Coulomb interaction increases. Theoretical and experimental work in this direction is mainly devoted to systems with a finite number of particles (excitons [1,2], trions [3,4], and electron-hole complexes with a number of particles less than 10 [5,6]).

The properties of a quasi-two-dimensional electron-hole liquid (EHL) in semiconductor structures are less studied. Recently, EHL has been detected in SiO₂/Si/SiO₂ quantum wells [7,8] and in Si/Si_{1-x}Ge_x/Si heterostructures [9-14] and GaAs/AlAs superlattices [15]. A fine structure in the photoluminescence spectra of the EHL in SiGe quantum wells with a small amount of Ge (several percent) both in the visible and in the infrared region was experimentally observed in [14]. It was possible to explain the shape of the condensed phase line within the framework of the concepts of a multicomponent Fermi liquid containing both heavy and light holes.

In this paper we use the density functional theory for finding the energy and the equilibrium density of a quasi-two-dimensional EHL with two types of holes. Three one-dimensional nonlinear Schrödinger equations are solved numerically for electrons, light and heavy holes.

2. Theoretical model

For quasi-two-dimensional EHL with electrons, heavy and light holes, the total energy is written as follows:

$$E_t[n_e, n_h] = T_e[n_e] + T_h[n_{hh}] + T[n_{hl}] + \frac{1}{2} \int V_c(z)(n_e(z) - n_h(z))dz + \int U_e(z)n_e(z)dz + \int U_{hh}(z)n_{hh}(z)dz + \int U_{hl}(z)n_{hl}(z)dz + E_{xc}[n_e, n_{hh}, n_{hl}] \quad (1)$$



where T_e , T_{hh} , T_{hl} are kinetic energy of electrons, heavy and light holes, respectively, $V_c(z)$ is the Coulomb potential, E_{xc} is the exchange-correlation energy, $U_e(z)$, $U_{hh}(z)$, $U_{hl}(z)$ are external potentials for electrons, heavy and light holes, respectively, n_e , n_{hh} , n_{hl} are density electron, heavy and light hole, respectively, $n_h = n_{hh} + n_{hl}$.

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

Varying expression (1) over the densities n_e , n_{hh} and n_{hl} , we obtain three Schrödinger equations:

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

where $i=e, hh, hl$.

Thus, the problem reduces to the solution of three one-dimensional nonlinear Schrödinger equations with potentials $V_{eff,e}(z) = V_c(z) + V_{xc,e}(z) + U_e(z)$, $V_{eff,hh}(z) = -V_c(z) + V_{xc,hh}(z) + U_{hh}(z)$ and $V_{eff,hl}(z) = -V_c(z) + V_{xc,hl}(z) + U_{hl}(z)$, where $V_{xc}(z)$ is the exchange-correlation potential, and the electrostatic potential is obtained from the Poisson equation:

$$V_c(z) = 8\pi \int_{-\infty}^z (z-z') [n_h(z') - n_e(z')] dz', \quad (3)$$

The external potentials for electrons and holes are given by the expression:

$$U_i(z) = \begin{cases} 0, & |z| \leq d/2 \\ V_i, & |z| > d/2 \end{cases}, \quad (4)$$

where d is the width of the well (barrier).

With this choice of external potentials, the energy is measured from the width of the SiGe band gap. The Si/SiGe transition is a type-II heterostructure, for which $V_e < 0$, $V_{hh} > 0$ and $V_{hl} > 0$. Due to deformations, the splitting of hole states occurs in the SiGe layer. The splitting of the valence band can be changed by applying a compensating pressure to the heterostructure. Below, the splitting between the heavy and light holes equals to zero.

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

$$n_e(z) = N_e \psi_{0,e}^2(z), \quad n_{hh}(z) = N_{hh} \psi_{0,hh}^2(z), \quad n_{hl}(z) = N_{hl} \psi_{0,hl}^2(z), \quad (5)$$

where N_e , N_{hh} , N_{hl} are two-dimensional electron, heavy and light hole densities, respectively.

Below, the index "0" at variables is omitted.

The kinetic energy has the following form:

$$T_i[n_i] = \frac{\pi\mu}{g_i m_{d,i}} N_i^2 + N_i (E_i - \int V_{eff,i}(z) \psi_i^2(z) dz). \quad (6)$$

In Eq. (6), the first term corresponds to the total kinetic energy of the carriers along the electron-hole layer, and the second corresponds to the kinetic energy across the layer.

For the exchange-correlation energy, we use the local density approximation:

$$E_{xc}[n_e, n_{hh}, n_{hl}] = \int dz e_{xc}(n_e, n_{hh}, n_{hl}), \quad (7)$$

where $e(n_e, n_{hh}, n_{hl})$ is the exchange-correlation energy of electrons and holes per unit volume.

Thus, the exchange-correlation potentials have the form:

$$V_{xc,e}(z) = \frac{de_{xc}}{dn_e}, \quad V_{xc,hh}(z) = \frac{de_{xc}}{dn_{hh}}, \quad V_{xc,hl}(z) = \frac{de_{xc}}{dn_{hl}}. \quad (8)$$

In general case, the form of the expression for e_{xc} is unknown. In the case of neutral EHL $n_e(z) = n_{hh}(z) + n_{hl}(z) = n(z)$ the approximation formula is available for the exchange-correlation energy $\varepsilon_{xc} = e_{xc}/n$ [16]:

$$\varepsilon_{xc} = \frac{1}{2} \frac{a + br_s}{c + dr_s + r_s^2}, \quad (9)$$

where $r_s = \left(\frac{3}{4\pi n}\right)^{1/3}$, $a = -4,8316$, $b = -5,0879$, $c = 0,0152$, $d = 3,0426$.

We consider an electrically neutral EHL, then $N_e = N_{hh} + N_{hl}$. Taking into account the Fermi energy of charge carriers with the density-of-states mass density $m_{d,i} = (m_{x,i}m_{y,i})^{1/2}$ and the number of equivalent valleys g_i is equal to $E_{F,i} = 2\pi\mu N_i / g_i m_{d,i}$ we have

$$E_{hh} + \frac{2\pi\mu N_{hh}}{g_{hh}m_{d,hh}} = E_{hl} + \frac{2\pi\mu N_{hl}}{g_{hl}m_{d,hl}}. \quad (10)$$

From Eq. (10) with $g_i=1$ for an electrically neutral EHL we obtain:

$$N_{hl} = N_e \frac{m_{d,hl}}{m_{d,hh} + m_{d,hl}} - \frac{m_{d,hh}m_{d,hl}}{m_{d,hh} + m_{d,hl}} \frac{E_{hl} - E_{hh}}{2\pi\mu}. \quad (11)$$

In case the expression (11) produces $N_{hl} < 0$, we take $N_{hh} = N_e$ and $N_{hl} = 0$.

Below, energy per electron-hole pair is measured from the energy level E_{hh} of heavy holes in the quantum well: $E_{eh} = -E_{hh} + E_F/N_e$.

3. Results

The system of nonlinear equations (2) - (11) was solved numerically. Calculations were carried out for the Si/SiGe/Si structure. For calculations, we used the following parameters [17, 18]: $V_e = 7,7x$, $V_{hh} = V_{hl} = 53,7x$, $g_e = 4$, $g_{hh} = g_{hl} = 1$, $m_{z,e} = 0,198m_0$, $m_{d,e} = 0,44m_0$, $m_{z,hh} = 0,28m_0$, $m_{d,hh} = 0,2m_0$, $m_{z,hl} = 0,18m_0$, $m_{d,hl} = 0,25m_0$, (m_0 is free electron mass). The calculations were carried out for a structure with a width of the well $d = 1$. The reduced mass has been taking from silicon $\mu = 0,126$, then $E_{ex} \approx 13\text{meV}$ and $a_{ex} \approx 5nm$.

The results of a numerical solution of the Schrödinger equations are shown in Fig. 1. The barrier causes the electron wave function to have a more extended state in comparison with the wave functions of the holes. Thus, holes create an attractive potential for electrons, which is more than twice the height of the barrier. Note that the exchange-correlation interaction also significantly reduces the height of the barrier for electrons.

Fig. 2 shows the dependence of the energy per one electron-hole pair on the two-dimensional density of pairs for different values of x . At $x = 0.03$, the equilibrium density of electron-hole pairs equal to 0.42 ($1.7 \cdot 10^{12} \text{ cm}^{-2}$), which is in a very good agreement with the experimental value [12,14]. With increasing x , the equilibrium density decreases and at $x=0.09$ it reaches the value of 10^{12} cm^{-2} . In this range EHL contains both heavy and light holes. Potential broadening at the heterointerfaces can be

accounted as in [19], but for the wide enough quantum well this correction is not of crucial effect on the electron-hole pair energy.

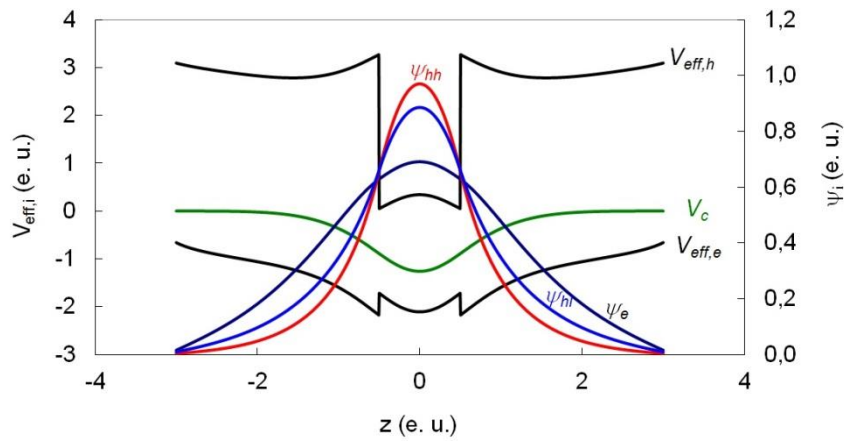


Figure 1. Profiles of wave functions and potentials for electrons, light and heavy holes ($N_e = 0.36$, $x = 0.06$).

The formation of EHL is possible if it is stable with respect to the decay into free excitons, that is, when the energy of the electron-hole pair, equal to $-E_{eh}$, is greater than the binding energy of the exciton. It was shown in [17, 20] that for $d > 1$ the binding energy of an exciton is close to the binding energy of a three-dimensional exciton. From the results presented in Fig. 2, it is seen that EHL binding energy is always over than 5 meV. The calculated binding energy is in good agreement with the experimental results [12, 14]. We note that the calculations for an EHL with heavy holes [21] give a much lower equilibrium density and binding energy.

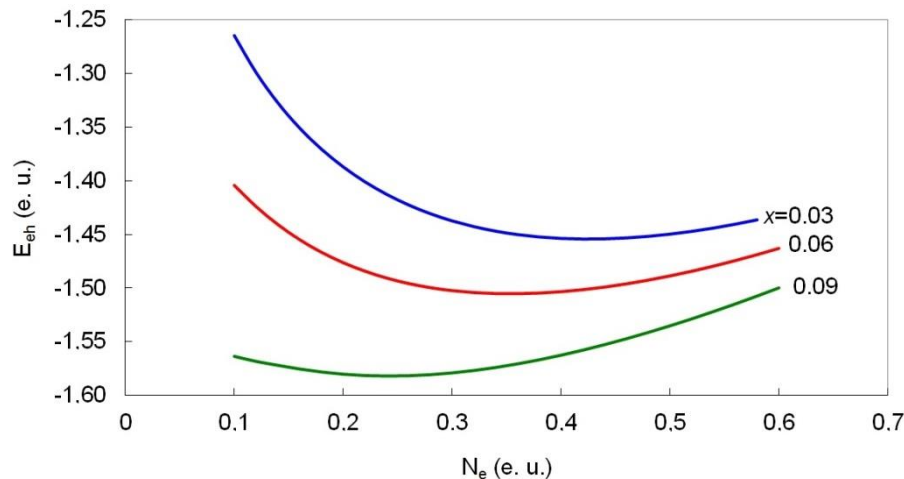


Figure 2. Dependence of the energy of an electron-hole pair on the two-dimensional density of electron-hole pairs.

At $x > 0.1$, there are only heavy holes in EHL (Fig. 3). This is due to the fact that as the well depth increases, the difference between the energy levels of light and heavy holes increases, and the potential energy of light holes outside the quantum well increases. EHL with heavy holes has a considerably lower equilibrium density than EHL with two types of holes. The decrease of equilibrium

density with increasing x is mainly due to the influence of the longitudinal kinetic energy, which is smaller in the SiGe layer for light holes.

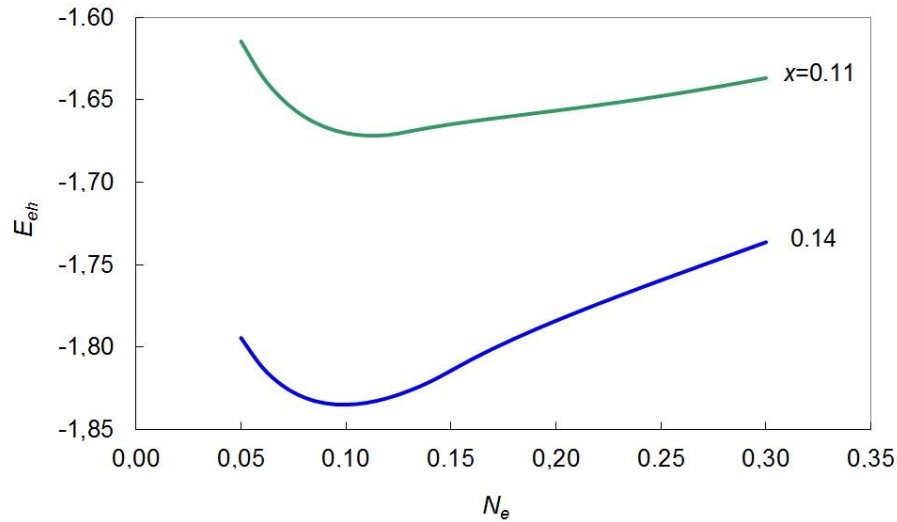


Figure 3. Dependence of the energy of an electron-hole pair on the two-dimensional density of electron-hole pairs.

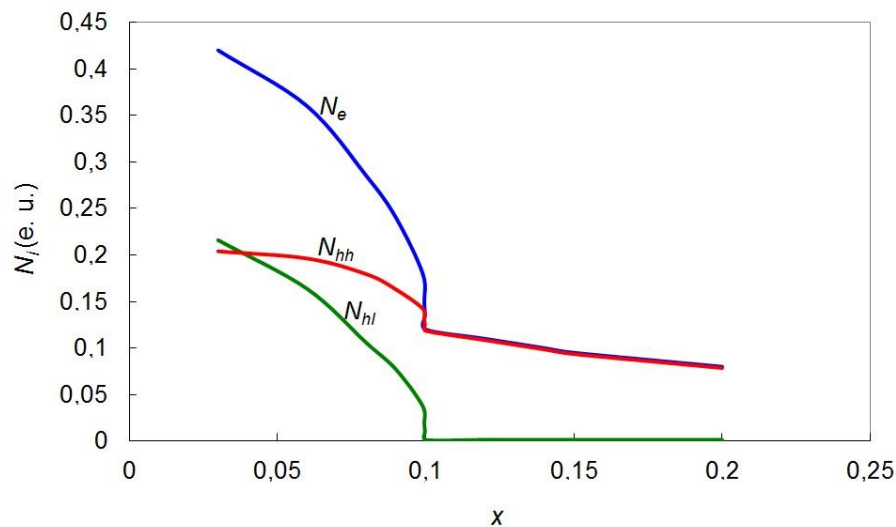


Figure 4. Dependence of two-dimensional densities of charge carriers on x .

Fig. 4 shows the dependence of the two-dimensional densities of charge carriers on Ge concentrations in the SiGe layer. It can be seen that for small x the densities of light and heavy holes are close. At $x > 0.1$ the EHL contains only heavy holes. Note that this transition occurs in structures with splitting of hole states at a much smaller value of x [22].

4. Conclusion

In this paper, we have calculated the EHL energy in the Si/Si_{1-x}Ge_x/Si quantum wells. It is shown that at low germanium concentrations, the EHL contains two types of holes. The minimum energy

corresponds to the equilibrium density of electron-hole pairs, for instance, at $x = 0.03$ the equilibrium density $N = 1.7 \cdot 10^{12} \text{ cm}^{-2}$. The calculated density agrees very well with the experimental results. With increasing x , a transition to a state with one type of hole occurs, and in this transition the density of electron-hole pairs decreases by more than three times. For $x > 0.1$, the EHL contains only heavy holes. Note that such a transition was observed in the experiment.

Acknowledgments

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