Ground state energy of the electron–hole liquid in type-II quantum wells

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Abstract

We present the ground state energy calculation of quasi-two-dimensional electron–hole liquid (EHL) at zero temperature in type-II quantum wells (QWs). The correlation energy is evaluated by random phase approximation of Hubbard. The effects of spatial separation of electrons and holes on the stability of EHL are explored by changing the distance between the QWs, taking extent of wave functions into account. Our calculated ground state energy of EHL for type-II GaAs/AlAs QWs is lower than the binding energy of exciton calculated recently so that it is expected that EHL should be more stable than exciton in type-II GaAs/AlAs QWs.

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1. Introduction

Semiconductor quantum wells (QWs) are representative artificial nanomaterial systems, and these have attracted our attention since the fabrication of heterostructure QWs lasers. It is known that the injected high-density electrons and holes play the key role in the laser action. The many-body effects on optical properties of QWs such as a band-gap renormalization and an appearance of quasi-two-dimensional (2D) electron–hole liquid (EHL) have been studied experimentally [1] and theoretically [2,3] in type-I QWs in which electrons and holes are located in the same confinement layers. A possible observation of the EHL in type-II GaAs/AlAs superlattices in which electrons and holes are located in different layers was reported by Kalt et al. [4] and Boujdaria et al. [5]. However, theoretical study of the liquid phase in type-II structures [6] is still scarce, because the estimation of correlation effects requires the numerous complicated computations.

In this paper we present the ground state energy calculation of quasi-2D EHL in type-II QWs with special emphasis on the effect of electron–hole (e–h) separation on the stability of the EHL. The correlation energy is evaluated by adopting random phase approximation (RPA) of Hubbard. The main difference of type-II QWs with type-I structure is the confinement of electrons and holes into the wells which are separated spatially. It may produce the characteristic contributions on the e–h correlation as well as the electrostatics. In order to demonstrate the non-local nature of such charge neutrality, we calculate the total energy as a function of pair density by changing the distance between wells with use of material parameters for GaAs/AlAs QWs.

This paper is organized as follows. In Section 2, energy formulae of the e–h system are described. In Section 3, the results and discussions are given. Section 4 is devoted to a brief summary.
The exchange energy for holes in Eq. (1),

\[ E_{\text{ex}} = \frac{1}{2} \left( \frac{\hbar^2 f_{\text{e}}^2}{2m_{\text{e}}} + \frac{\hbar^2 f_{\text{h}}^2}{2m_{\text{h}}} \right), \]

where \( f_{\text{h}} \) (\( f_{\text{e}} \)) is the Fermi wave number of hole (electron) and \( m_{\text{h}} \) (\( m_{\text{e}} \)) is hole (electron) effective mass. To connect the present model to type-II GaAs/AlAs QWs, it is assumed that the electron exchange energy is an ellipsoid of revolution, so \( m_{\text{e}} = \sqrt{m_{\text{e},xy}m_{\text{e}}}, \)

\( m_{\text{e},xy} \) being the longitudinal and transverse mass, respectively. The exchange energy per e–h pair \( E_{\text{ex}} \) in Eq. (1) is

\[ E_{\text{ex}} = E_{\text{ex}}^{(e)} + E_{\text{ex}}^{(h)}. \]

The exchange energy for holes \( E_{\text{ex}}^{(h)} \) is given by

\[ E_{\text{ex}}^{(h)} = -N^{-1}(2\pi)^{-4} \int_{\mathbb{R}^4} d\mathbf{k} d\mathbf{l} v_{\text{hh}}(|\mathbf{k} - \mathbf{l}|), \]

where \( v_{\text{hh}}(q) \) denotes the Fourier component of Coulomb interaction between holes. The Fourier components of Coulomb interaction between \( i-j \) particles will be written by

\[ v_{ij}(q) = \frac{2\pi e^2}{\epsilon q} \int_{-\infty}^{+\infty} dz \int_{-\infty}^{+\infty} dz' e^{-q |z-z'|} |\psi_i(z)|^2 |\psi_j(z')|^2 \]

with dielectric constant \( \epsilon \) and the wave function of the lowest subband \( \psi_i(z) \). The exchange energy \( E_{\text{ex}}^{(e)} \) has the similar form with Eq. (4), but the Fermi surface of electron is an ellipse

\[ \hbar^2 f_{\text{e}}^2/2m_{\text{e},z} + \hbar^2 f_{\text{e}}^2/2m_{\text{e},xy} = \hbar^2 f_{\text{e}}^2/2m_{\text{e}}. \]

Thus, the integrals over \( \mathbf{k} \) can be done by transforming \( \mathbf{k} \) to \( \mathbf{k} \) as

\[ \hat{k}_i = \kappa^{-1/4} k_{x_i}, \quad \hat{k}_y = \kappa^{1/4} k_{y_i}, \]

with \( \kappa = m_{\text{e,xy}}/m_{\text{e,z}} \).

In bulk and type-I structure, the Hartree energy is diminishingly small because of the local charge neutrality between electrons and holes. But in type-II structure, this energy plays important role. The Hartree energy \( E_{\text{H}} \) with the charge density \( \rho(z) \) and electrostatic potential \( \phi(z) \) becomes

\[ E_{\text{H}} = (2N)^{-1} \int_{-\infty}^{+\infty} dz \phi(z) \rho(z), \]

where

\[ \rho(z) = -eN(|\psi_e(z)|^2 - |\psi_h(z)|^2) \]

and \( \phi(z) \) is obtained by solving the Poisson’s equation.

We will evaluate the correlation energy \( E_{\text{C}} \) for type-II QWs by adopting RPA of Hubbard [7]

\[ E_{\text{C}} = \frac{\hbar}{4\pi^2 N} \int_{0}^{\infty} q \, dq \int_{0}^{\infty} d\omega \int_{0}^{1} \frac{d\lambda}{\lambda} \]

\[ \times \left\{ \frac{\beta - \alpha T}{\alpha^2 + \beta^2} + \nu_{ee}(q) \Sigma_e(q, \omega) \lambda + \nu_{hh}(q) \Sigma_h(q, \omega) \lambda \right\}, \]

where

\[ \alpha = 1 + \{(G_e - 1)\nu_{ee} A_e + (G_h - 1)\nu_{hh} A_h\} \lambda \]

\[ + \{(1 - G_e)(1 - G_h)\nu_{ee} v_{hh} - \nu_{eh}\} \times (A_e A_h - \Sigma_e \Sigma_h) \lambda^2, \]

\[ \beta = \{(G_e - 1)\nu_{ee} \Sigma_e + (G_h - 1)\nu_{hh} \Sigma_h\} \lambda \]

\[ + \{(1 - G_e)(1 - G_h)\nu_{ee} v_{hh} - \nu_{eh}\} \times (A_e \Sigma_e + A_h \Sigma_h) \lambda^2, \]

\[ S = (\nu_{ee} A_e + \nu_{hh} A_h) \lambda + \{(G_e + G_h - 2)\nu_{ee} v_{hh} + 2 \nu_{eh}\}(A_e A_h - \Sigma_e \Sigma_h) \lambda^2, \]

\[ T = (\nu_{ee} \Sigma_e + \nu_{hh} \Sigma_h) \lambda + \{(G_e + G_h - 2)\nu_{ee} v_{hh} + 2 \nu_{eh}\}(A_e \Sigma_e + A_h \Sigma_h) \lambda^2. \]

In Eqs. (10) and (11), \( A_i \) and \( \Sigma_i \) are the real and imaginary parts of 2D polarizability in the RPA, respectively, as

\[ A_i(q, \omega) = \frac{m_i}{\pi \hbar^2 q} \left[ \left( \frac{m_i \omega}{\hbar q} + \frac{q}{2} \right) \sqrt{1 - \left( \frac{2\hbar f_i q}{2m_i \omega - \hbar q^2} \right)^2} - \left( \frac{m_i \omega}{\hbar q} - \frac{q}{2} \right) \sqrt{1 - \left( \frac{2\hbar f_i q}{2m_i \omega - \hbar q^2} \right)^2} - q \right], \]
\[ \Sigma_i(q, \omega) = \frac{m_i}{\hbar^2 q} \left[ \sqrt{1 - \left( \frac{m_i \omega}{\hbar q} + \frac{q}{2} \right)^2} - \sqrt{1 - \left( \frac{m_i \omega}{\hbar q} - \frac{q}{2} \right)^2} \right], \]

where \( \sqrt{1 - x^2} \) is defined as \( x < 0 \). \( G_i(q) \) \( (i = e, h) \) denotes the so-called exchange correction suggested by Hubbard [7] as

\[ G_i(q) = \nu_i \left( \frac{q^2 + f_i^2}{2} \right) / 2v_0(q). \]

In the above \( E_C \), we account \( e-e, h-h \) and \( e-h \) correlation effects in the RPA of Hubbard. So far, the exchange correction for \( e-h \) system is done for \( \Sigma_e + \Sigma_h \) and \( A_e + A_h \) because the Coulomb interactions are approximated by the same form, and the integral over \( \lambda \) was evaluated easily [2]. However, since in the present case \( v_j \) \((i, j = e, h)\) differ each other, these remain in the integration over \( \lambda \).

Finally we define the minimum in \( E_{\text{tot}} \) vs \( e-h \) pair density as the EHL ground state energy \( E_\text{G} \) per \( e-h \) pair, i.e.,

\[ E_\text{G} = \min \{E_{\text{tot}}(N)\}. \]

3. Results and discussion

The appearance of the EHL in type-II GaAs/AlAs QWs is expected much because of the spatial separation of electron and hole, in addition to their indirect nature of energy gap in k-space as in Ge. Such favorable condition to observe the EHL stimulates intensive photoluminescence experimental studies under high excitations [4,5]. Here, apart from experiments we focus on the entire energy calculation of the EHL for our modeled type-II QWs according to formulae in Section 2. In order to compare previous theoretical results in type-I QWs, we depicted the results as a function of \( r_s \) instead of pair density. The parameter \( r_s \) is defined as

\[ r_s = \frac{1}{a_B \sqrt{\pi N}}, \]

with the Bohr radius \( a_B = (\epsilon \hbar^2 / e^2)[m_e^{-1} + (m_{e,x} + m_{e,y}) / 2]. \) As was emphasized in Section 1, we will elucidate the role of \( e-h \) separation in determination of \( E_{\text{tot}} \) because the spatial separation of electrons and holes is characteristic in type-II QWs. For this purpose, we assume that electrons and holes are confined in the AlAs QW and the GaAs QW, respectively. Then, we employ the important parameters of systems such as \( L = 2.83 \text{ nm}, \ m_{e,z} = 1.1 m_0, \ m_{e,x,y} = 0.19 m_0, \ m_h = 0.51 m_0, \ e = 11.17, \ V_e = 300 \text{ meV}, \ V_h = 550 \text{ meV}. \) The Bohr radius is estimated to be \( a_B = 2.98 \text{ nm}. \)

In Fig. 2 we plot \( E_{\text{tot}} \) as a function of \( r_s \) for \( d = 0 \) (a), 1.41 (b), 2.83 (c), 5.65 (d) and 8.84 nm (e). Fig. 2 contains the binding energy of the exciton \( B_X \) in (GaAs)$_{10}$(AlAs)$_{10}$ type-II superlattice calculated recently [8]. As is seen in Fig. 2, the type-I QWs \((d = 0 \text{ nm})\) exhibit quite large \( E_\text{G} \), while \( E_\text{G} \) is reduced much by increasing \( d \). If \( r_0 \) is the \( r_s \) corresponding to the equilibrium density which is determined by the location for minimum of \( E_{\text{tot}} \), we can see that \( r_0 \) moves from \( r_0 \approx 1 \) to 1.8 as \( d \) is increased from 0 to 8.84 nm. In Fig. 3 we plot \( E_{\text{kin}} + E_X \) and \( E_H \) as a function of \( r_s \) for the same \( d \)'s in Fig. 2 to investigate the origin of the change of \( r_0 \). We can see that \( E_H \) exhibits a strong dependence on \( d \) while \( E_{\text{kin}} + E_X \) does not change as \( d \) is increased. For short \( d \), the local charge distribution associated with electrons and holes cancels out each other due to a requirement of charge neutrality. But when the distance \( d \) becomes large, electrons and holes are confined in each well so that the \( E_H \) becomes large in the high-density regime.

![Fig. 2. The total energy \( E_{\text{tot}} \) vs \( r_s \) for \( d = 0 \) nm (a), \( d = 1.41 \) nm (b), \( d = 2.83 \) nm (c), \( d = 5.65 \) nm (d) and \( d = 8.48 \) nm (e). The horizontal dashed line indicates the calculated exciton binding energy \( B_X \) in (GaAs)$_{10}$(AlAs)$_{10}$ type-II superlattice [8].](image)

![Fig. 3. The Hartree energy \( E_H \) vs \( r_s \) for \( d = 0 \) nm (a), \( d = 1.41 \) nm (b), \( d = 2.83 \) nm (c), \( d = 5.65 \) nm (d) and \( d = 8.48 \) nm (e). The kinetic energy plus the exchange energy \( E_{\text{kin}} + E_X \) is also plotted.](image)
This contribution gives rise to significant decrease of equilibrium density in competition with $E_{\text{kin}} + E_X$ as $d$ is increased. To demonstrate the effects of e–h separation on correlation energy, we plot $E_C$ as a function of $r_s$ for several $d$ in Fig. 4. It is seen that $|E_C|$ becomes small when $d$ is increased from 0 to 8.84 nm. This indicates that e–e and h–h correlation effects do not change, but e–h correlation is reduced much for the large e–h separation.

For the stability problem, the EHL will be formed if the ground state energy of EHL is lower than the energy of exciton (or excitonic molecule). It is evident that the ground state energy of the EHL for $d = 2.83$ nm is lower than the binding energy of the exciton as is seen in Fig. 2. Thus, it indicates that the EHL is more stable than the exciton in type-II (GaAs)$_{10}$(AlAs)$_{10}$ QWs.

4. Concluding remarks

We have presented the ground state energy calculation of quasi-2D EHL at zero temperature in type-II QWs. The correlation energy is evaluated by adopting the RPA of Hubbard. The reduction of the EHL ground state energy occurs due to the large separation of electrons and holes in consequence of that the Hartree energy becomes large whereas the correlation energy is reduced. In type-II (GaAs)$_{10}$(AlAs)$_{10}$ QWs, we expected that the EHL is more stable state than exciton at high density condition. Though the effects of e–h separation on the Coulomb energies are explored in the modeled type-II QWs, such structure will be realized by fabricating appropriate QWs which have the band structure as shown in Fig. 1.

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Fig. 4. The correlation energy $E_C$ vs $r_s$ for $d = 0$ nm (a), $d = 1.41$ nm (b), $d = 2.83$ nm (c), $d = 5.65$ nm (d) and $d = 8.48$ nm (e).