Exchange-induced terahertz minigap in InAs/GaSb type II and broken-gap quantum wells

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We theoretically demonstrate that the exchange effect induced by the carrier-carrier interaction can cause the hybridization of the electron and hole dispersion relations in InAs/GaSb-based type II and broken-gap quantum well (QW) systems. As a result, a terahertz minigap at the anticrossing point of the conduction and valence bands can be induced by the interlayer electron-hole coupling via the Coulomb interaction. It is shown that the many-body effect is another important source of the hybridization of the dispersion relations in InAs/GaSb QW systems. © 2008 American Institute of Physics. [DOI: 10.1063/1.2913757]

In InAs/GaSb-based type II and broken-gap quantum well (QW) systems, the top of the valence band in the GaSb layer can be significantly higher than the bottom of the conduction band in the InAs layer. As a result, both electron and hole subbands in different well layers can be populated so that the conducting electrons and holes are spatially separated in two adjacent layers. It is both experimentally and theoretically found that in such QWs, due to the coupling of the conduction and valence bands in different material layers, the electron and hole dispersions along the two-dimensional (2D) plane are hybridized and a minigap at the anticrossing point between the electron and hole dispersion relations is observed. For typical sample structures, the value of this minigap is found to be of the order of several meV or 1 THz. The presence of this minigap can produce a semiconducting rather than a semimetallic behavior of the device systems. In particular, experimental and theoretical works have shown that the presence of a hybridization minigap is responsible for the giant negative magnetoresistance in InAs/GaSb type II QWs. This indicates that from both a fundamental research and a device application point of view, it is necessary and important to investigate the hybridization of the dispersion relations in such QW systems.

The hybridization of the electron and hole dispersion relations in InAs/GaSb QW systems can be normally examined using, e.g., a k·p band-structure calculation. Such calculation is essentially a single-particle approach in which the coupling between different electron bands is included through kinetic interactions. In an InAs/GaSb broken-gap QW, both electron and hole states are occupied and new channels, therefore, open up for many-body interaction, especially for the interlayer electron-hole interaction via the Coulomb potential due to the overlap of the electron and hole wave functions at the InAs/GaSb interface. Thus, the strength of the many-body interaction in a type II QW system is considerably enhanced. As a result, the many-body effects such as the carrier-carrier (c-c) interaction via the Coulomb potential can play a crucial role in determining the electronic subband structure of the system. In this study, we examine how many-body effects such as the exchange interaction can affect the hybridization of the electron and hole dispersion relations in InAs/GaSb-based type II and broken-gap QWs.

In the model, we consider that (1) the growth direction of the QW is along the z axis, (2) the 2D electron gas (2DEG) and the 2D hole gas (2DHG) are formed in different layers in the xy plane, and (3) only the lowest electron sub-band in the InAs layer and the highest heavy-hole subband in the GaSb layer are occupied. Under the usual effective-mass approximation, the electron \( j = e = 2 \) and hole \( j = h = 1 \) wave functions and energy spectra can be written, in the absence of electronic scattering centers and band hybridization, as

\[
\Psi_{j}(R) = e^{i k R} \psi_0(z) \quad \text{and} \quad E_{j} = (-1)^{j} \frac{\hbar^2 k^2}{2m_j} + \epsilon_0^j,
\]

where \( R = (r, z) = (x, y, z) \), \( k = (k_x, k_y) \) is the wave vector for an electron or a hole in the 2D plane, \( m^* \) is the electron/hole effective mass, and the ground-state subband wave function \( \psi_0(z) \) and energy \( \epsilon_0^j \) are determined by Schrödinger equations for an electron and a hole along the growth direction. By applying the electron and hole wave functions and the energy spectra to the usual random-phase approximation (RPA), the RPA dielectric function matrix is obtained as

\[
e(\Omega, q) = \begin{bmatrix}
1 - A_{ee} & A_{eh} \\
A_{he} & 1 - A_{hh}
\end{bmatrix},
\]

where \( A_{jj'}(\Omega, q) = \sum_{l} \tilde{V}_{q} F_{jj'}(q) \Pi_{jj'}(\Omega, q) \) is induced by a scattering of an electron or a hole in layer \( j \) to layer \( j' \), \( \Omega \) is the excitation frequency, \( \tilde{V}_{q} = 2 \pi e^2/(\kappa_{x} q) \) with \( \kappa_{x} \) being the static dielectric constant for material layer \( j \), and \( q = (q_x, q_y) \) is the change of the carrier wave vector in the 2D plane during a c-c scattering event, \( F_{jj'}(q) = \int dz_1 \int dz_2 |\psi_0(z_1)|^2 |\psi_0(z_2)|^2 e^{-i \mathbf{r} \cdot \mathbf{r}'} \) is a form factor for c-c scattering in a 2D system, and \( \Pi_{jj'}(\Omega, q) \) is the usual density-density correlation function.

With the single-particle wave functions for an electron and a hole given by Eq. (1), the two-particle Slater wave functions are formed through

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where $\Psi^{\mu}_{k_{1}}(R_1, R_2) = C(\Psi_{k_{1}}^{\mu}(R_1)\Psi_{k_{1}}^{\nu}(R_2) - \Psi_{k_{1}}^{\nu}(R_1)\Psi_{k_{1}}^{\mu}(R_2))]$,

\begin{equation}
\Psi^{\mu}_{k_{1}}(R_1, R_2) = C(\Psi_{k_{1}}^{\mu}(R_1)\Psi_{k_{1}}^{\nu}(R_2) - \Psi_{k_{1}}^{\nu}(R_1)\Psi_{k_{1}}^{\mu}(R_2)),
\end{equation}

with $C = 1/\sqrt{2}$. The electrostatic energy induced by the c-c scattering via the Coulomb potential $V(R) = e^2/(|k_j|R)$ is then

$E_{d_{ij}} = \langle k_{1} \rangle|\Psi_{k_{1}}^{\mu}(R_1)\Psi_{k_{1}}^{\nu}(R_2) - \Psi_{k_{1}}^{\nu}(R_1)\Psi_{k_{1}}^{\mu}(R_2))| = U_{d_{ij}}^0 - U_{d_{ij}}^E$. Here, the first term arises from the Hartree scattering $U_{d_{ij}}^0 = \lim_{q \to 0} \sum_{j} V_{q} F_{jj}(q)$ and the second term arises from the exchange scattering $U_{d_{ij}}^E = \delta_{k_{1},k_{1}+q} V_{q} F_{jj}(q)$, where the momentum conservation for the c-c scattering has been taken into account. The effective scattering energy for Hartree $(\alpha = H)$ and exchange $(\alpha = E)$ interactions in the presence of c-c screening can be calculated through $U_{d_{ij}}^\alpha = \epsilon_{d_{ij}}(q)U_{d_{ij}}^\alpha$, where $\epsilon_{d_{ij}}(q) = \lim_{q \to 0} \epsilon_{d_{ij}}(q, j, k)$ is the element of the static dielectric function matrix [see Eq. (2)]. In the presence of the c-c screening, the Hartree self-energy provides only a constant energy background. We therefore neglect the effect of the Hartree interaction and pay attention only to those effects induced by the c-c scattering. At low temperatures (i.e., $T \to 0$), the exchange self-energy in the presence of the c-c screening is calculated via

\begin{equation}
\Xi_{d_{ij}}(k) = -\sum_{k' < k} \frac{2\pi e^2}{\kappa_j |q + K_{d_{ij}}(q)|} \delta_{q + k, k'}.
\end{equation}

Here, $k_{d_{ij}}$ is the Fermi wave vector for an electron or a hole and $K_{d_{ij}}(q)$ is the RPA inverse screening length for different scattering channels. In general, different c-c scattering processes have different screening lengths. Because the strongest effect of the RPA screening on exchange self-energy occurs at $q \to 0$, in the present study, we include the effect of the c-c screening at the long-wavelength limit in order to reach a simple analytical result. When $q \to 0$, $\lim_{q \to 0} K_{d_{ij}}(q) = K_{d_{ij}}$, where

\begin{equation}
K_{d_{ij}} = K_{d_{ij}} - \frac{2\alpha e^2}{\hbar^2 \kappa_j (m_e^* + m_h^*)} \frac{M^2}{M},
\end{equation}

with $M = [\ln(m_e^*/m_h^*)]^{m_e^*/m_h^* + m_h^*/m_e^*}$.

Applying the exchange self-energy induced by the c-c interaction to the diagrammatic techniques, the Green’s function for a many-body quasiparticle in an electron-hole bilayer system is represented as

\begin{equation}
G_{d_{ij}}(E, k) = [E - G^{-1}_j(E, k) - \Xi_{d_{ij}}(k)]^{-1},
\end{equation}

where $G_j(E, k) = E - E^j_+ + i\delta$ is Green’s function for an electron or a hole in the absence of the c-c interaction, with $E$ being the electron/hole energy. In the form of a matrix, Eq. (6) becomes

\begin{equation}
G_{d_{ij}}(E, k) = \frac{1}{B_{d_{ij}} + iB_1 \delta} \left[ E_+ - \Xi_{d_{ij}}(k) \right] = E_{\pm} - \Xi_{d_{ij}}(k),
\end{equation}

where

\begin{equation}
E_{\pm} = E_+ - \Xi_{d_{ij}}(k), \quad B_{d_{ij}} = E_+(E, k)E_-(E, k).
\end{equation}

Thus, we obtain a live many-body quasiparticle with an energy dispersion determined by the poles of Green’s function $B_{d_{ij}} = 0$, which reads

\begin{equation}
E_{\pm} = E_+ - \Xi_{d_{ij}}(k) \Xi_{d_{ij}}(k), \quad B_{d_{ij}} = E_+(E, k)E_-(E, k). \end{equation}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure1.png}
\caption{Dependence of the exchange self-energy on carrier wave vector for different interaction channels. The results are for an InAs/GaSb QW with the well widths $L_{inhv} = 17$ nm and $L_{GaSb} = 5$ nm. Here, $\Xi_{d_{ij}}$ stands for scattering from layer $j$ to layer $j'$, $\Delta = 2\sqrt{\Xi_{d_{ij}}(k)}$ is the energy gap, and $k_{d_{ij}}$ is the Fermi wave vector for an electron. Note that the exchange self-energy $\Xi_{d_{ij}} < 0$ [see Eq. (4)].}
\end{figure}

\begin{equation}
E_{\pm}(k) = \frac{1}{2}\left[ E^L_+ + \Xi_{d_{ij}}(k) + E^L_0 \right]
\end{equation}

\begin{equation}
+ \Xi_{d_{ij}}(k) \Xi_{d_{ij}}(k) = \sqrt{\left[ E^L_+ + \Xi_{d_{ij}}(k) - E_b^L - \Xi_{d_{ij}}(k) \right]^2 + \Delta^2},
\end{equation}

where $\Delta = 2\sqrt{\Xi_{d_{ij}}(k)\Xi_{d_{ij}}(k)}$ is a $k$-dependent energy gap. Equation (8) is very similar to that previously proposed for the hybridized band structure in a type II QW. We see that when the many-body interaction is present, the energy gap between hybridized energy spectra is caused by interlayer electron-hole coupling via the Coulomb interaction.

In the present study, we consider a typical InAs/GaSb QW in which the type II and broken-gap structure can be experimentally achieved. The widths of the InAs and GaSb well layers are taken, respectively, to be $L_{inhv} = 17$ nm and $L_{GaSb} = 5$ nm. We calculate the electronic subband structure by self-consistently solving the Schrödinger and Poisson equations. The results obtained from this calculation are electron density $n_e = 9.0 \times 10^{11}$ cm$^{-2}$, hole density $n_h = 1.4 \times 10^{11}$ cm$^{-2}$, $e^0_v = 52.0$ meV, and $e^0_h = 111.1$ meV measured from the bottom of the conduction band in the InAs layer. In such a structure, only the lowest electron subband and the highest heavy-hole subband are occupied, respectively, by electrons and heavy holes. Furthermore, in the calculation, we use the material parameters $m_e^* = 0.038m_e$, $m_h^*$, $m_e$, and $m_h$ being the rest electron mass, $m_e^*$, and $m_h^*$, respectively, and $\kappa_e = 15.15$, $\kappa_h = 15.69$. The results are obtained and presented for the case of low temperature ($T \to 0$).

In Fig. 1, we show the exchange self-energy for different c-c scattering channels as a function of carrier wave vector in an InAs/GaSb QW. We see that the absolute value of $\Xi_{d_{ij}}(k)$ decreases with increasing wave vector $k$ and, as a result, the energy gap $\Delta = 2\sqrt{\Xi_{d_{ij}}(k)\Xi_{d_{ij}}(k)}$ decreases with increasing $k$. This behavior is similar to that obtained from the $k \cdot p$ calculations. For a type II QW with $L_{inhv} = 17$ nm and $L_{GaSb} = 5$ nm, the Fermi level of the system is very close to the top of the highest heavy-hole subband. This is also experimentally implied by a relatively low hole density in the samples. The Fermi wave vector for electrons $k_{d_{ij}}$ is therefore much larger than that for holes $k_{d_{ij}}$. Together with the fact that an electron has a much lower effective mass than a heavy...
hole has, the electron-electron interaction is stronger than the hole-hole interaction and $|E_{ee}|>|E_{eh}|>|E_{eh}|>|E_{hh}|$, as shown in Fig. 1. In Fig. 2, we show the energy dispersion relations $E_x(k)$ for a quasiparticle induced by exchange scattering (solid curves) in an InAs/GaSb QW. The results are compared to those obtained in the absence of the $c\cdot c$ interaction $E_x(k)$ (dashed curves). From Fig. 2, we note the following features. (i) As in the case of a conventional QW, exchange scattering via the Coulomb interaction in a type II QW can lower the energy of the system. For $L_{InAs}=17$ nm and $L_{GaSb}=5$ nm, because $|E_{ee}|>|E_{eh}|>|E_{eh}|>|E_{hh}|$ (see Fig. 1), the reduction of the system energy is more pronounced for the electronlike branch $E_x(k)$ and depends on the wave vector $k$. (ii) In the presence of exchange interaction in an InAs/GaSb QW, the hybridization of the electron and hole dispersion relations can be clearly observed. The presence of this kind of band hybridization is a consequence of the many-body interaction. (iii) A minigap is clearly located at the anticrossing points of the energy spectra for a many-body quasiparticle. For a typical sample structure with well widths $L_{InAs}=17$ nm and $L_{GaSb}=5$ nm, the exchange-induced minigap at the anticrossing points is found to be about 6 meV or 1.5 THz, in agreement with those obtained from the experimental measurements and from the self-consistent $k\cdot p$ calculations.\(^1\)

In a type II and broken-gap QW, the electron-hole interactions via interlayer scattering mechanism can occur due to the penetration of the electron and hole wave functions to different well layers.\(^8\) The exchange-induced energy gap therefore depends on the self-energies induced by electron-hole scattering channels. Hence, from a physics point of view, the hybridization of the electron and hole dispersions induced by the exchange effect via the $c\cdot c$ interaction differs from that observed in the $k\cdot p$ calculations. It should be noted that although the $k\cdot p$ calculation is a single-particle approach, interactions between different bands are implied through the inclusion of the kinetic interactions. This is the main reason why the features of exchange-induced band hybridization in an InAs/GaSb QW are quite similar to those obtained from the $k\cdot p$ calculations. The most important conclusion we draw from this study is that the many-body effects, such as the exchange scattering induced by the $c\cdot c$ interaction via the Coulomb potential, is another major source of the hybridized band structure in InAs/GaSb-based type II and broken-gap QW systems. The present study is based on the usual plane wave and parabolic energy spectrum for the 2DEG/2DHE in a type II QW. A complete calculation should start from the eigenstates obtained from the $k\cdot p$ Hamiltonian\(^3\) and use the $k\cdot p$ results as the bases to evaluate the $c\cdot c$ interactions. In such a way, the band hybridization induced by the kinetic interactions between the conduction and valence bands in different layers can also be included. However, this considerably requires more analytical and numerical work, and we, therefore, do not attempt it here. In contrast to the $k\cdot p$ results, the band hybridization induced by pure exchange interaction in an InAs/GaSb type II QW takes a simple analytical form, as shown in this study. From these simple results, we can gain a deeper physical understanding of the electronic subband structure in InAs/GaSb-based type II and broken-gap QW systems.

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