PHYSICAL REVIEW B, VOLUME 65, 201305(R)

Many-body effects in a laterally inhomogeneous semiconductor quantum well

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(Received 28 December 2001; revised manuscript received 8 February 2002; published 8 May 2002)

Many-body effects on conduction and diffusion of electrons and holes in a semiconductor quantum well are studied using a microscopic theory. The roles played by the screened Hartree-Fock (SHF) terms and the scattering terms are examined. It is found that the electron and hole conductivities depend only on the scattering terms, while the two-component electron-hole diffusion coefficients depend on both the SHF part and the scattering part. We show that, in the limit of the ambipolar diffusion approximation, however, the diffusion coefficients for carrier density and temperature are independent of electron-hole scattering. In particular, we found that the SHF terms lead to a reduction of density-diffusion coefficients and an increase in temperature-diffusion coefficients. Such a reduction or increase is explained in terms of a density- and temperature-dependent energy landscape created by the band-gap renormalization.

DOI: 10.1103/PhysRevB.65.201305 PACS number(s): 72.10.Bg, 73.63.Hs, 71.35.Ee

Our understanding of Coulomb interaction in an optically excited semiconductor has been greatly enriched recently thanks to the extensive theoretical[1–3] and experimental investigations[4] over the past few decades. As far as optical properties in highly excited semiconductors (with high carrier density) are concerned, many-body effects manifest themselves in two important ways: the renormalization of the single-particle energies and the finite lifetime of such renormalized single-particle states. Though quantitative calculation of these two quantities is still a topic of current research, the qualitative difference of these two features seems to be quite clear. For the sake of convenience of the presentation in this paper, we classify the two types of terms into coherent and incoherent (or scattering) parts, since the renormalization of single-particle state changes the resonance frequency, while scattering leads to a decay of coherence or oscillation. For a spatially uniform system, these two types of effects manifest themselves in the linear optical spectrum and have received extensive attention in the past decades. The manifestation of the many-body effects in a spatially nonuniform system has not received comparable attention, with Ref. 5 being the only paper dealing with the effects of Coulomb interaction on diffusion process up to now, to the best of our knowledge. It is especially interesting to see, as we will show later, that these two parts of many-body interaction play different roles in the conduction and diffusion processes in a spatially nonuniform semiconductor.

In this communication, we report on our recent theoretical study on the effects of many-body interaction in a spatially inhomogeneous system. The starting point of our investigation is the set of Boltzmann-Bloch-Poisson equations, which contains many-body interactions in the spirit of Refs. 1–3 and 6. Namely, the coherent part is treated within the screened Hartree-Fock (SHF) approximation, while the carrier scatterings are treated within the second Born approximation. Among many other scattering channels only LO-phonon scatterings are included in this model study. After following the standard moment equation approach[7] by assuming the quasiequilibrium distribution of carriers, a set of coupled diffusion equations for carrier densities and temperatures can be derived[8] and given as follows:

$$\partial_t N^\alpha + \partial_{\vec r}\cdot \vec J_N^\alpha = R_N^\alpha, \tag{1}$$

$$\partial_t T^\alpha + \partial_{\vec r}\cdot \vec J_T^\alpha - j_W^\alpha \vec u^\alpha \cdot \partial_{\vec r} W^\alpha + \partial_{\vec r} j_N^\alpha \cdot \vec J_N^\alpha - \partial_{\vec r} j_W^\alpha \cdot \vec J_W^\alpha = R_T^\alpha, \tag{2}$$

where N^α, W^α, $\vec u^\alpha$, and T^α stand for density, thermal energy, drift velocity, and temperature of electrons $(\alpha=e)$ or holes $(\alpha=h)$. The temperature equations are obtained through $\partial_t T^\alpha = j_W^\alpha \partial_t W_\alpha - j_N^\alpha \partial_t N_\alpha$. $j_W^\alpha = 1/(\partial W^\alpha/\partial T^\alpha)|_{N^\alpha}$ and $j_N^\alpha = \partial W^\alpha/\partial N^\alpha|_{T^\alpha}/(\partial W^\alpha/\partial T^\alpha)|_{N^\alpha}$ are transform Jacobians. In Eqs. (1) and (2), R_N^α's represent generation and recombination of carriers due to pumping and optical transitions, while R_T^α's represent the corresponding heat sources or sinks, which include, in particular, the energy relaxation due to carrier-phonon scatterings. The density and thermal currents in Eqs. (1) and (2) are given by

$$\vec J_N^\alpha = \frac{\vec P^\alpha}{m_\alpha}, \tag{3}$$

$$\vec J_T^\alpha = j_W^\alpha \vec J_W^\alpha - j_N^\alpha \vec J_N^\alpha = \left(2 j_W^\alpha \frac{W^\alpha}{N^\alpha} - j_N^\alpha \right) \vec J_N^\alpha, \tag{4}$$

where m_α's are the effective masses. $\vec P^\alpha$'s stand for two-dimensional (2D) momentum densities, and thus $\vec J_N^\alpha$ are number current densities, which can be written in terms of gradients of the four macroscopic variables $(X = N^e, N^h, T^e, T^h)$ and the electrical potential Φ as[8]

$$\vec J_{N^\alpha} = -\sum_X D_{N^\alpha X} \partial_{\vec r} X - \frac{\sigma^\alpha}{q^\alpha} \partial_{\vec r} \Phi, \tag{5}$$

where we have introduced various diffusion coefficients and conductivities[8] $(\alpha \neq \beta)$:

$$D_{N^\alpha N^\alpha} = \chi_\alpha [(1+\eta_\alpha)(C_{N^\alpha}^\alpha + H_{N^\alpha}^\alpha) + H_{N^\alpha}^\beta], \tag{6}$$

$$D_{N^\alpha N\beta} = \chi_\alpha [(1+\eta_\alpha) H_{N\beta}^\alpha + H_{N\beta}^\beta + C_{N\beta}^\beta], \tag{7}$$

$$D_{N^\alpha T^\alpha}=\chi_\alpha[(1+\eta_\alpha)(C^\alpha_{T^\alpha}+H^\alpha_{T^\alpha})+H^\beta_{T^\alpha}], \tag{8}$$

$$D_{N^\alpha T^\beta}=\chi_\alpha[(1+\eta_\alpha)H^\alpha_{T^\beta}+H^\beta_{T^\beta}+C^\beta_{T^\beta}], \tag{9}$$

$$\sigma^\alpha=\chi_\alpha e^2[N^\alpha(1+\eta_\alpha)-N^\beta]. \tag{10}$$

Following two shorthand notations have been introduced:

$$C^\alpha_X=\partial_X W^\alpha, \tag{11}$$

$$H^\alpha_X=N^\alpha\partial_X\delta\epsilon^\alpha. \tag{12}$$

Obviously, the C^α_X's are specific heats of a certain kind, which represent the contribution from free electron and hole gases, while H^α_X's are the contributions due to many-body interaction, as they are proportional to the derivatives of self-energy renormalization[2] ($\delta\epsilon^\alpha$) with respect to densities or temperatures. While Eqs. (6)–(9) define diffusion coefficients in the density currents (noting the first index of the coefficients being N^α), the corresponding diffusion coefficients in the thermal currents are defined through the relation between the density currents J^α_N and thermal currents J^α_T, Eq. (4). Factors χ_α and η_α in Eqs. (6)–(10) are defined as follows:

$$\chi_\alpha=\left[\frac{\gamma^e_{LO}\gamma^h_{LO}}{\gamma^\beta_{e\text{-}h}}(m_e+m_h)+(m_e\gamma^e_{LO}+m_h\gamma^h_{LO})\right]^{-1}, \tag{13}$$

$$\eta_\alpha=\frac{\gamma^\beta_{LO}}{\gamma^\beta_{e\text{-}h}}\frac{m_e+m_h}{m_\alpha}, \tag{14}$$

where $\alpha\neq\beta$. γ^α_{LO} and $\gamma^\alpha_{e\text{-}h}$ are the relaxation rates of the α-component momentum due to carrier-LO (c-LO) phonon and due to electron-hole (e-h) scattering, respectively. These rates are defined microscopically in Ref. 8.

Several general features can be readily observed from the expressions in Eqs. (6)–(10): First, all diffusion coefficients and conductivities depend on momentum relaxation rates due to e-h scattering through factors χ_α and η_α. On the other hand, the coherent part of the many-body interaction (through H^α_X) only enters the diffusion coefficients, but not the conductivities. Second, it is interesting to consider the ambipolar diffusion coefficients, as commonly defined by setting equal the density currents of electrons and holes. The ambipolar currents are now written as[8]

$$\vec{J}_N=-D_{NN}\partial_{\vec{r}}N-D_{NT}\partial_{\vec{r}}T, \tag{15}$$

$$\vec{J}_T=-D_{TN}\partial_{\vec{r}}N-D_{TT}\partial_{\vec{r}}T, \tag{16}$$

with

$$D_{NX}=\frac{C^e_X+C^h_X}{m_e\gamma^e_{LO}+m_h\gamma^h_{LO}}+\frac{H^e_X+H^h_X}{m_e\gamma^e_{LO}+m_h\gamma^h_{LO}}\equiv D^0_{NX}+\Delta D_{NX}, \tag{17}$$

$$D_{TX}=\left[2j_w\frac{W}{N}-j_N\right]D_{NX}\equiv D^0_{TX}+\Delta D_{TX}, \tag{18}$$

where $X=N,T$ as we also assumed the densities and temperatures to be the same for the two components. The identity in Eq. (17) defines the free-carrier diffusion coefficient D^0_{NX} and the corresponding many-body correction ΔD_{NX}. We observe that the e-h scattering rate $\gamma^\alpha_{e\text{-}h}$ (the incoherent part of the many-body effects) disappears from the ambipolar diffusion coefficients completely. Only c-LO phonon scattering rates γ^α_{LO}'s remain. This means that the ambipolar diffusion coefficients depend only on the weighted sum of the scattering rates of electrons and holes with LO phonons. The coherent part of the many-body interactions, however, remains present in the ambipolar diffusion coefficients, as expressed by the second terms ΔD_{NX} and ΔD_{TX} in Eqs. (17) and (18), respectively. The absence of the e-h scattering and the remaining presence of the coherent part of the Coulomb interaction in the ambipolar diffusion coefficients clearly illustrate different roles played by the two aspects of the same Coulomb interaction. We note that the absence of the e-h scattering in the ambipolar diffusion coefficients is also implied in Ref. 5. But unlike the situation here, all the Coulomb interaction terms drop out from the diffusion coefficient in Ref. 5 completely including the coherent part under the ambipolar diffusion approximation. The absence of the e-h scattering can be easily understood, since such scattering represents collisions of the electrons and holes, which now are parts of integral entities diffusing together under the ambipolar diffusion approximation. However, the coherent part creates a new density- and temperature-dependent environment (energy landscape) for the original quasiparticles (with unrenormalized energies). They diffuse in the modified energy landscape, resulting in an effective change in diffusion coefficients, as we will explain in more detail in the following.

To study more quantitatively the effects of the coherent part of the many-body interaction, we examine the relative change in diffusion coefficients as defined by $\delta D_{XY}=\Delta D_{XY}/D^0_{XY}$. In Figs. 1–4, we plot δD_{XY} (a) and D_{XY} (b) with respect to density for all four ambipolar diffusion coefficients. As a model material, we use a quasi-2D GaAs of 8 nm in width modified by a form factor. Only one subband each from the conduction and valence bands is considered. All the material parameters are standard and will not be listed. Figure 1 shows the familiar density-diffusion coefficient D_{NN}. In Fig. 1(b), coefficients D_{NN} (solid lines) and D^0_{NN} (dashed lines) are plotted versus carrier density at three temperatures. The rapid rise around 10^{12} cm^{-2} is mainly due to the statistical degeneracy and will be explained in more detail in a regular paper.[9] We see that the coherent many-body effects result in a reduction in the diffusion coefficient. The relative change of diffusion coefficient is plotted in Fig. 1(a), where we see a diffusion coefficient reduction of over 25% at 200 K. This reduction decreases as temperature increases. Similar behavior is also observed in Fig. 2 for the mutual-diffusion coefficient D_{TN}, which relates carrier density gradient to thermal flux $\vec{J}_T$. Figure 3 shows the temperature-diffusion coefficient D_{TT} and D^0_{TT} (a)

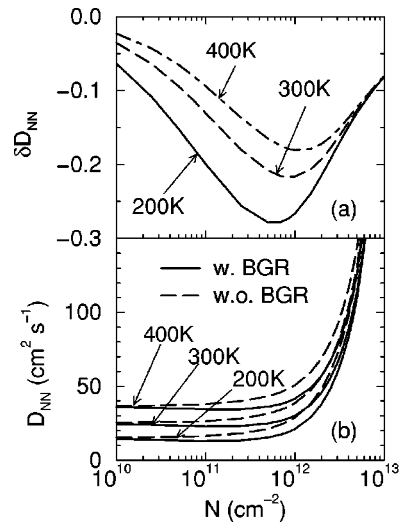

FIG. 1. Diffusion coefficient D_{NN} (b) and its relative change δD_{NN} (a) versus carrier density at three temperatures as indicated. Solid and dashed curves in (b) are for D_{NN} and D^0_{NN}, respectively.

and the corresponding relative change δD_{TT}. Contrary to the reduction of diffusion coefficients shown in Figs. 1 and 2, we see an increase in D_{TT}, i.e., $D_{TT} > D^0_{TT}$. Furthermore, the relative increase δD_{TT} is much smaller in magnitude than δD_{NN} and δD_{TN} in Figs. 1 and 2. The change is less than 10%. Similar behavior is shown in Fig. 4 for the mutual-diffusion coefficient D_{NT}, which describes carrier density flux induced by the temperature gradient.

Let us now explain these figures in more detail. We begin with the reduction in diffusion coefficients, D_{NN} and D_{TN}, in Figs. 1 and 2, both of which are determined by the derivatives with respect to density [see Eqs. (11), (12), (17), and (18)]. This reduction can be explained by the band-gap renormalization. We note that D_{NN} describes a carrier density flux from high-density region to low-density region. Due to

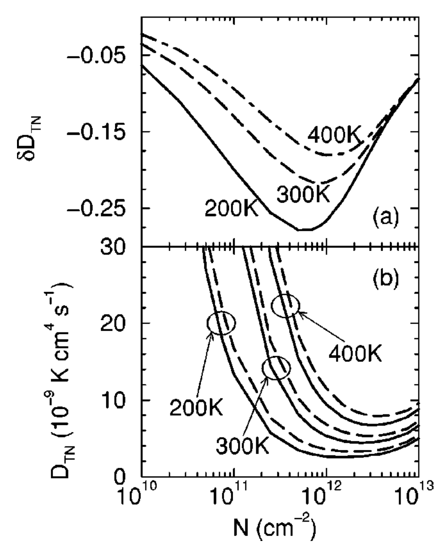

FIG. 2. Diffusion coefficient D_{TN} (b) and its relative change δD_{TN} (a) versus carrier density at three temperatures as indicated. Solid and dashed curves in (b) are for D_{TN} and D^0_{TN}, respectively.

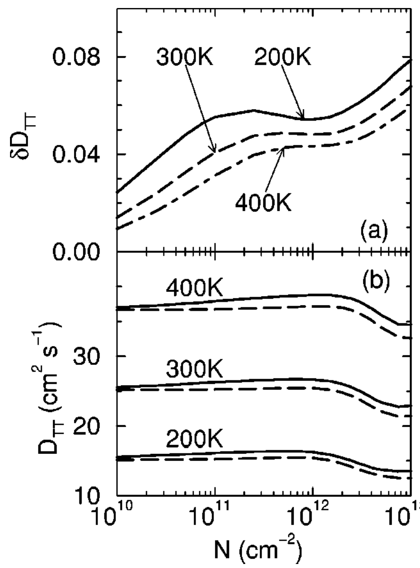

FIG. 3. Diffusion coefficient D_{TT} (b) and its relative change δD_{TT} (a) versus carrier density at three temperatures as indicated. Solid and dashed curves in (b) are for D_{TT} and D^0_{TT}, respectively.

band-gap renormalization, which increases with carrier density, the high-density region has a smaller total band gap than the low-density region. This means that a diffusing particle from high-density region to low-density region will have to climb an uphill energy landscape due to many-body effects, thus leading to a reduction in the effective diffusion coefficients. The reduction in the mutual-diffusion coefficient D_{TN} needs slightly different explanation. First, we note that D_{TN}, by definition, describes the *thermal* flux from high-*density* region to low-density region. Due to the band-gap renormalization, an energy band-gap profile is created. A thermal flux is therefore induced from the high band-gap (lower density) region to a lower band-gap (higher density) region to coun-

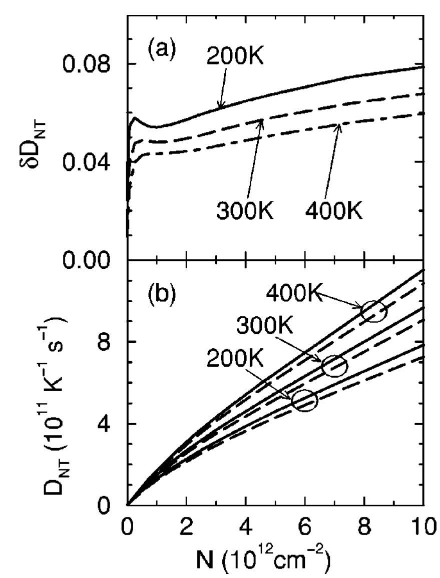

FIG. 4. Diffusion coefficient D_{NT} (b) and its relative change δD_{NT} (a) versus carrier density at three temperatures as indicated. Solid and dashed curves in (b) are for D_{NT} and D^0_{NT}, respectively.

teract the thermal flux and to equilibrate the total energy (band gap plus the thermal energy) profile. The situations described in Figs. 3 and 4 are exactly the reverse of that in Figs. 1 and 2. The increase in the diffusion coefficients is due to the band-gap renormalization that decreases with plasma temperature[10] instead of increasing with density as in Figs. 1 and 2. The energy landscape reverses from the cases of Figs. 1 and 2 and leads to an increase of diffusion coefficients D_{NT} and D_{TT}. In short, the many-body effects on diffusion coefficients lead to a decrease in those diffusion coefficients that are related to the density gradient (D_{NN} and D_{TN}) and an increase in those that are related to temperature gradient (D_{TT} and D_{NT}). Finally, the smaller change in D_{TT} and D_{NT} (Figs. 3 and 4) than in D_{NN} and D_{TN} (Figs. 1 and 2) is due to the weaker dependence of the band-gap renormalization with respect to plasma temperature than to density.

Another feature of Figs. 1 and 2 is the decrease of the relative change δD_{NN} and δD_{TN} at lower densities until the carrier density reaches the critical value near 1×10^{12} cm^{-2}, where electrons become degenerate. This decrease is a result of the reduction of the band gap due to band-gap renormalization and an almost constant value of D_{NN} and D_{TN}. The relative change δD_{NN} reaches a minimum around 28% for 200 K. With the further increase of carrier density, δD_{NN} and δD_{TN} start to increase as the carriers become strongly degenerate and D^0_{NN} and D^0_{TN} begin to rise dramatically.[9] At high density for lasing over 1×10^{12} cm^{-2}, the diffusion reduction is still over 20%. The larger values of δD_{NN} and δD_{TN} at higher temperatures are mainly due to the increase of the D^0_{NN} and D^0_{TN} with temperature.

In summary, many-body effects are investigated in a semiconductor quantum well where spatial nonuniformity of densities and temperatures exists along the quantum well plane. Different roles played by the coherent and incoherent parts of Coulomb interaction are analyzed. While both coherent and incoherent parts contribute to the diffusion coefficients of the general two-component system, the conductivities depend only on the scattering part. Even though e-h scattering plays an important role in legitimizing the ambipolar diffusion approximation,[8] we show that the diffusion coefficients of the established composite system do not depend on the e-h scattering rate. Instead the ambipolar diffusion coefficient depends only on the coherent part of the interaction, the band-gap renormalization. We found that the coherent many-body interaction leads to a significant reduction of the ambipolar diffusion coefficients D_{NN} and D_{TN} and an increase in coefficients D_{TT} and D_{NT}. We note that this quite significant change in diffusion coefficients, especially in D_{NN} and D_{TN}, should be important in describing optoelectronic devices where spatial inhomogeneities of densities, or plasma temperatures occur. Such nonuniformities are quite ubiquitous in high power and ultrafast devices,[11] such as lasers, photoconductors, and photodetectors. Simulations of such devices using the microscopically calculated diffusion coefficients will be reported elsewhere.

The authors thank Rolf Binder for a helpful discussion on the diffusion coefficient reduction.

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