Temperature and carrier-density dependent excitonic absorption spectra of semiconductor quantum wires (Postprint)

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Abstract

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Full Text

Preamble

Temperature and Carrier-Density Dependent Excitonic Absorption Spectra of Semiconductor Quantum Wires

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We present a theoretical study on excitonic absorption spectra of one-dimensional semiconductor quantum wires. Carrier-carrier scattering is treated using the second Born approximation in the Markovian limit. The absorption spectra at various carrier densities and temperatures are discussed. The

excitonic absorption peak position and width exhibit complicated dependence on carrier density and temperature, indicating the importance of carrier-carrier scattering. This behavior can be understood through the cooperative effects of exchange self-energy and Coulomb correlation arising from carrier-carrier scattering.

Keywords: Semiconductor quantum wire, Exciton, Absorption, Carrier-carrier scattering
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Introduction

Semiconductors are important materials for nuclear science and technology and have been widely used in radiation detection. Both theoretical and experimental studies have shown increasing interest in low-dimensional semiconductor structures in recent years. In the longer term, compound semiconductors may be used as radiation detectors with higher performance and without strain limitations. Thus, research on the properties of low-dimensional semiconductors is of great importance.

Semiconductor quantum wires (QWRs), in which electrons and holes are confined in one direction, represent typical one-dimensional (1D) systems. State-of-the-art QWR structures have been realized experimentally using molecular beam epitaxy with cleaved edge overgrowth and growth-interrupt annealing techniques.

In semiconductors, excitons are quasi-particles that form when electrons and holes become bound through Coulomb interactions. In 1D semiconductor structures, quantum confinement makes excitonic effects on optical spectra more pronounced than in three- and two-dimensional structures. The signatures of excitons appear in the optical absorption spectra of direct-gap semiconductors such as GaAs, showing a sharp peak several meV below the band gap energy.

Many-body effects play important roles in light-semiconductor interactions, including excitonic nonlinearity, band-gap renormalization (BGR), and Coulomb screening. These complex many-body phenomena can be revealed through optical spectra. In a typical experiment involving simultaneous measurements of absorption and photoluminescence (PL) spectra, peaks induced by excitons at low carrier density and by plasma at very high density have been observed.

It is therefore necessary to apply reasonable many-body theory to understand the observed features in the optical spectra of QWRs. Under the Hartree-Fock approximation, the Semiconductor Bloch Equations (SBEs) are sufficient for calculating excitonic nonlinearity, phase-space filling, and band gap renormalization. However, the absorption line width in SBEs is treated merely as a phenomenological input parameter with carrier-carrier scattering neglected. Thus, a theory describing carrier-carrier scattering in a higher-order approximation is needed.

In this paper, we apply a theoretical method based on quantum kinetic equations. Carrier-carrier scattering is treated using the second Born approximation (SBA) in the Markovian limit.

Model and Numerical Method

In our scheme, the quantum kinetic equation for microscopic polarization p_k is given by

$$i(cid:126)\frac{\partial p_k}{\partial t} = (cid:126)\omega'_k p_k - (cid:126)\Omega_k(1-f_{ek}-f_{hk}) - i(cid:126)\Lambda_{kk}p_k + i(cid:126)\sum_{k'(cid:54)=k}\Lambda_{kk'}p_{k'}$$

where $(cid:126)\omega = \epsilon_{ek}+\epsilon_{hk}+\Delta_k+E_{g0}$ is the renormalized transition energy, ω' is the renormalized transition frequency, and k is the corresponding wavevector. The exchange self-energy contribution to the renormalized band gap energy is

$$\Delta_k = -\sum_{k'} V_{|k-k'|}(f_{ek'} + f_{hk'}).$$

The renormalized Rabi energy is

$$(cid:126)\Omega_k = d_{c\nu}\tilde{\varepsilon}_0 \exp(-i\omega t) + \sum_{k'(cid:54)=k} V_{|k'-k|}p_{k'}.$$

In Eqs. (1)-(4), k is the momentum, $(cid:126)$ is Planck's constant, ϵ_{ek} and ϵ_{hk} are the single-particle energies of electrons and holes. The band gap energy at zero carrier density is defined as E_{g0}. V is the effective Coulomb potential. In 1D systems, the Coulomb interaction is treated as an effective interaction by averaging the three-dimensional Coulomb interactions over the electron and hole wave functions along the lateral directions. The distribution functions of electrons and holes are defined as f_{ek} and f_{hk}. Under quasi-equilibrium conditions, both distribution functions can be described by Fermi-Dirac functions and are nearly time-independent. $d_{c\nu}$ is the dipole matrix element between electrons and holes. $\tilde{\varepsilon}_0$ and ω are the amplitude and frequency of the electric field component of the applied optical field. Carrier-carrier scattering gives rise to the last two terms on the right-hand side of Eq. (1), which can be divided into diagonal $(cid:126)\Lambda_{kk}$ and non-diagonal terms $(cid:126)\Lambda_{kk'}$.

The diagonal and non-diagonal contributions due to carrier-carrier scattering are

$$(cid:126)\Lambda_{kk} = \sum_{k''}\sum_{q(cid:54)=0}\sum_{a,b=e,h}(2V_S^2(q)-\delta_{a,b}V_S(q)V_S(k-k''+q))\times g(\delta\epsilon)[f_{a,k+q}(1-f_{b,k''})f_{b,k''-q}+(1-f_{a,k+q})$$

$$(cid:126)\Lambda_{kk'} = \sum_{k''} \sum_{a,b=e,h} (2V_S^2(q) - \delta_{a,b} V_S(q) V_S(k-k''+q)) \times g(-\delta\epsilon)[(1-f_{a,k})(1-f_{b,k''}) f_{b,k''-q} + f_{a,k} f_{b,k''}(1-f_{b,}$$

where $q = k' - k$, $V_S(q) = V(q)/\varepsilon_q$ is the screened potential, with ε_q being the static dielectric function using the Lindhard formula in the plasmon-pole approximation. $\delta_{a,b}$ is the Kronecker delta function and $g(\delta\epsilon) = \lim_{\nu\to 0} i/(\delta\epsilon + i\nu)$ is the Heitler-Zeta function, with $\delta\epsilon = \epsilon_{ak} + \epsilon_{bk'} - \epsilon_{ak+q} - \epsilon_{bk'-q}$ and ν being a small constant.

To solve Eq. (1) numerically, we convert it to the numerical solution of the equation for microscopic susceptibility

$$\sum_{k'} ((cid:126)\omega\delta_{kk'} - H^{\text{eff}}_{kk'})\chi_{k'}(\omega) = -(1 - f_{ek} - f_{hk}) d_{c\nu}.$$

The effective Hamiltonian is denoted as

$$H^{\text{eff}}_{kk'} = (\epsilon_{ek} + \epsilon_{hk} + \Delta_k + E_{g0})\delta_{kk'} - (1 - f_{ek} - f_{hk}) V_{|k-k'|} - i(cid:126)\Lambda_{kk}\delta_{kk'} + i(cid:126)\Lambda_{kk'}.$$

The absorption coefficient can be calculated by

$$\alpha(\omega) \propto \text{Im} \sum_k \frac{|d_{c\nu}|^2 \sum_{k'} \phi^{L*}_{jk'}(1 - f_{ek'} - f_{hk'})}{(cid:126)\omega - E_j} \phi^R_{jk},$$

where ϕ^L_{jk} and ϕ^R_{jk} are the j-th left and right eigenvectors corresponding to the effective Hamiltonian $H^{\text{eff}}_{kk'}$, and E_j is the j-th eigenvalue. The symbol Im means taking the imaginary part of a complex function. Since the effective Hamiltonian is complex, the eigenvalues and eigenvectors are complex numbers and complex vectors, respectively. Unlike the situation at the Hartree-Fock level, no phenomenological damping parameter is needed here. The absorption line width is attributed to the imaginary part of E_j.

Numerical calculations are carried out for a typical rectangular cross-section GaAs quantum wire with the following parameters: $E_{g0} = 1.5$ eV, dielectric constant $\varepsilon_0 = 13.74$, cross-section length $l_x = 14$ nm and width $l_y = 6$ nm, and $d_{c\nu} = 4.33$ e • Å. The effective masses of electrons and holes are $m_e = 0.0665 m_0$ and $m_h = 0.457 m_0$, where m_0 is the free electron mass.

Results and Discussion

Figure 1 [Figure 1: see original paper] shows the calculated absorption spectra of the GaAs QWR for different carrier densities at $T = 60$ K and different temperatures at $n_e = n_h = 0.2 \times 10^6$ cm^{-1}. A strong absorption peak about 20 meV below the band gap is ascribed to excitons. In Fig. 1(a), the intensity of the excitonic peak decreases with increasing carrier density, while the peak position energy remains nearly constant. In contrast, SBE theory predicts a large red shift in the excitonic absorption peak with increasing carrier density, which can be understood as an overestimation of band gap renormalization. The present approach shows a constant excitonic absorption peak, which agrees well with experimental results. Since an exciton is an electrically neutral quasi-particle, the Coulomb interaction has little dependence on carrier density, resulting in constant exciton energy. At a carrier density of $n_e = n_h = 0.2 \times 10^6$ cm^{-1}, when the temperature increases, the excitonic absorption peak shows a red shift. Moreover, the peak width increases with temperature, indicating stronger carrier-carrier scattering at higher temperatures. Systematic micro-PL measurements on a QWR have shown the stability of the excitonic peak, providing good support for our theoretical results.

Figure 2 [Figure 2: see original paper] shows data for the peak position energy at $T = 60$ K (Fig. 2(a)) and at a carrier density of $n_e = n_h = 0.2 \times 10^6$ cm^{-1} (Fig. 2(b)). Each error bar in the minus and plus direction denotes the lower and upper half-widths of the peak. At a constant temperature of 60 K, the peak energy changes little and the peak width increases only slightly as the carrier density varies. At a constant carrier density of $n_e = n_h = 0.2 \times 10^6$ cm^{-1}, the peak energy decreases with increasing temperature. Therefore, temperature affects the excitonic absorption peak energy more than carrier density does.

For direct-gap semiconductors, the band gap is defined as the energy difference between the conduction and valence bands at $k = 0$, i.e., the center of the Brillouin zone. Figure 3 [Figure 3: see original paper] shows the exchange self-energy Λ_k at $k = 0$ for temperature $T = 60$ K (Fig. 3(a)) and carrier density $n_e = n_h = 0.2 \times 10^6$ cm^{-1} (Fig. 3(b)). The energy depends differently on carrier density and temperature. As contributions from carrier-carrier scattering (Eqs. (5) and (6)) are considered, the imaginary parts of diagonal and non-diagonal terms add additional energy shifts to the band gap. The exchange self-energy, together with the energy shift from scattering and the exciton binding energy, ultimately determines the excitonic peak position and width, as shown in Fig. 2.

Conclusion

In conclusion, we have performed a theoretical study on the absorption spectra of a GaAs QWR at different carrier densities and temperatures. The excitonic absorption peak position and width exhibit complicated behaviors as temperature or carrier density varies. This can be understood through the cooperative effects of exchange self-energy and Coulomb correlation due to carrier-carrier scattering.

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Note: Figure translations are in progress. See original paper for figures.