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Microscopic theory for the valence intersubband absorption of quantum wells

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Abstract

In this paper we focus on the temperature dependence and on a detailed analysis of the interplay between Coulomb effects at Hartree–Fock level, namely: subband shifts, exchange and depolarization shifts to the valence intersubband absorption of III–V semiconductor quantum wells. We show how the tendency of the depolarization to create double peaks in the absorption spectra in the presence of a strongly k-space localized dipole moment can be partially compensated by the other Coulomb corrections considered.

Keywords: Quantum cascade lasers; Many body effects; Intersubband transitions

1. Introduction

Since the initial proposal of quantum cascade lasers, [1] and their actual experimental realization, [2] intersubband absorption spectra are an important research topic at the moment, both from a basic physics point of view, as well as for prospective application in mid-infrared and terahertz spectroscopy [3–6,8–10]. In a recent paper we have discussed the Coulomb and valence band effects in a combined valence and conduction band excitation scheme. In this paper, we focus on one of the spectra and consider in detail the contribution of each Coulomb correction at the Hartree–Fock level and clearly pin-point the double feature that develops in the low-energy side as a consequence of the depolarization shift [7].

2. Main equations

The optical absorption α at a given photon energy $\hbar\omega$ can be calculated from the imaginary part of the optical susceptibility,

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$$\alpha(\omega) = \frac{4\pi\omega}{cn_b}\Im\{\chi(\omega)\},$$
$$\chi(\omega) = \frac{2}{\Omega}\sum\nolimits_{\mu\neq v,\vec{k}} d_{\mu v}\chi_{v,\mu}(k,\omega). \quad (1)$$

Here n_b denotes the background refractive index, c is the speed of light, Ω is the sample volume; $d_{v\mu}$ is the transition. The transition dipole moment between subbands v and μ, which are labelled $v = 1,2,\ldots$ from the top valence band. Thus in the discussion of numerical results that follows, absorption of a photon of light with an electron being promoted from subband $\mu = 2$ to $v = 1$ is called a $(2,1)$ transition.

The optical susceptibility is related to the carriers Green's function. It is beyond the scope of this short paper to give full derivations of the Green's functions equations, and their connection to the optical response. Further details for intersubband optics can be found in [6,7], while more complete derivations for the case of interband transitions, further including luminescence and laser output power and their connection to the photon Green's function are given in [11,12].

In the Hartree–Fock regime, it reads

$$\left[\hbar\omega - e_{v\mu k} + i\Gamma_{v\mu}\right]\chi_{v\mu}(k,\omega) - \delta f_{v\mu k}\sum\nolimits_{\mathbf{k}'\neq\mathbf{k}}\chi_{v\mu}(k',\omega)\tilde{V}^{v\mu}_{\mathbf{k}-\mathbf{k}'} = d_{v\mu}\delta f_{v\mu k}, \quad (2)$$

where

$$\tilde{V}^{v\mu}_{\mathbf{k}-\mathbf{k}'} = V\begin{pmatrix} vv\mu\mu \\ \mathbf{k}-\mathbf{k}' \end{pmatrix} - 2V\begin{pmatrix} v\mu\mu v \\ 0 \end{pmatrix}.$$

The population difference is given by $\delta f_{v\mu}(\mathbf{k}) = f_v(\mathbf{k}) - f_\mu(\mathbf{k})$. The bare Coulomb interaction matrix elements read

$$V\begin{pmatrix} \mu v\lambda\beta \\ \mathbf{k}-\mathbf{k}' \end{pmatrix} = \int \mathrm{d}z\,\mathrm{d}z'\phi^*_\mu(z)\phi_v(z) \times \frac{2\pi e^2\exp(-|\mathbf{k}-\mathbf{k}'||z-z'|)}{\epsilon_0|\mathbf{k}-\mathbf{k}'|}\phi^*_\lambda(z')\phi_\beta(z'), \quad (3)$$

and ϵ_0 denotes the background dielectric constant.

$$e_{v\mu}(\mathbf{k}) = E_v(\mathbf{k}) - E_\mu(\mathbf{k}) - \sum\nolimits_{\mathbf{k}'} f_v(\mathbf{k}')V\begin{pmatrix} vvvv \\ \mathbf{k}-\mathbf{k}' \end{pmatrix} + \sum\nolimits_{\mathbf{k}'} f_\mu(\mathbf{k}')V\begin{pmatrix} \mu\mu\mu\mu \\ \mathbf{k}-\mathbf{k}' \end{pmatrix} + \sum\nolimits_{\mathbf{k}'}[f_v(\mathbf{k}') - f_\mu(\mathbf{k}')]V\begin{pmatrix} v\mu\mu v \\ \mathbf{k}-\mathbf{k}' \end{pmatrix}, \quad (4)$$

is the energy difference between the levels renormalized by the exchange interaction, which we refer to as the subband shift in the following.

3. Numerical results and discussion

The numerical results that follow are for a 5-nm $GaAs/Al_{0.3}Ga_{0.7}As$ quantum well at 300 K. Material parameters used are given in Table 1. Our numerical technique can be summarized as follows:

The starting point is the diagonalization of an 8×8 $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian. The momentum operator is calculated consistently with the Hamilton operator by evaluating the k-gradient [13]. For quantum wells, the components of the k-vector parallel to the growth direction are replaced by the corresponding symmetrized spatial derivatives as outlined in [14].

Next, for a given carrier density, the equilibrium (Fermi) occupation functions, Coulomb matrix elements, dephasing rates, and renormalized energies are evaluated. Eq. (2) is then discretized leading to a system of linear equations which is solved for each photon frequency. A final numerical integration and summation over all possible

Table 1
Parameters used for the computation of the band structure

Parameter	Symbol	Quantum well	Barriers
Average valence band energy	E_{v0}/eV	0.171	0
Energy gap	E_g/eV	1.425	1.842
Spin–orbit splitting energy	Δ/eV	0.34	0.322
Energy equivalent of momentum matrix element	E_p/eV	26.10	26.08
Luttinger parameter	γ_1	6.85	5.77
Luttinger parameter	γ_2	1.65	1.35
Luttinger parameter	γ_3	2.35	2.01

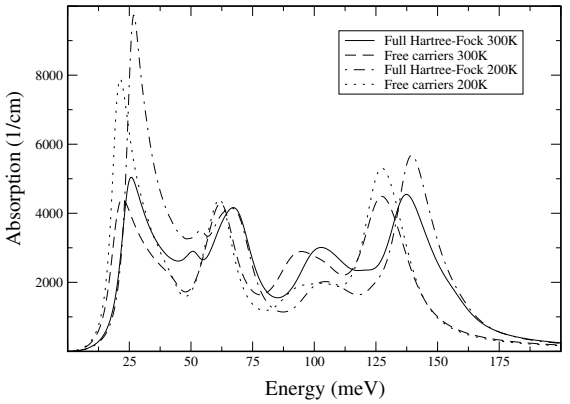

Fig. 1. TE valence band absorption of a 5-nm GaAs/AlGaAs quantum well with a carrier density $N = 3 \times 10^{12}/\mathrm{cm}^2$.

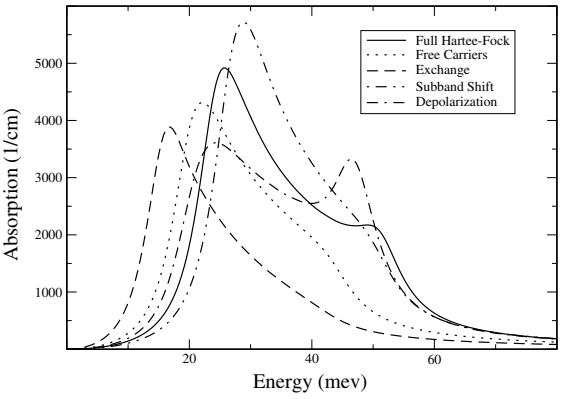

Fig. 2. Different many-body contributions to the valence intersubband absorption between the two first valence subbands, denoted (2, 1) transition (see main text) for the same conditions of Fig. 1.

intersubband transitions yields the final optical spectra (Eq. (1)). K-space is partitioned in sections between 0 and a maximum value $K_{\max}$ and the density of k points is doubled until the resulting numerical inversion and integrations converge. A total of either 100 or 200 k-points suffices for calculations with temperatures between 200 and 300 K.

The valence subband transitions dominate the TE optical spectra for the III–V quantum wells considered here, and in Fig. 1 we show a comparison between the valence intersubband absorption with all many-body effects at Hartree–Fock and for free carriers for two different temperatures. As the temperature is reduced, the smaller dephasing combined with higher occupation of the lowest subband at quasi-equilibrium leads to higher oscillator strength, but the positions of the spectral peaks are not changed. However, they do change when many-body effects are considered, since the different spectral shifts and oscillator strength redistribution is strongly temperature dependent.

In Fig. 2 we show how each different many-body correction combines with the strong valence band nonparabolicity. The origin of the double peak into which the (2, 1) transition evolves can be ascribed to the depolarization shift. The depolarization has the tendency of shifting the spectral peak to the blue. However, not all k-space can be effectively spanned, since the transition dipole moment is strongly localized. Consequently, instead of a full shift, only a partial redistribution of oscillator strength occurs leading to a double-peaked structure. When we consider all other corrections, there is a compensation of this effect. The double feature would not be pronounced if only the depolarization would be present.

In summary, by analyzing the influence of each many-body correction to the valence intersubband absorption of III–V semiconductor quantum wells we have shown how the tendency of the depolarization to create double peaks in the absorption spectra in the presence of a strongly localized dipole moment can be partially compensated by the other Coulomb effects at Hartree–Fock level. We hope that our numerical predictions will stimulate further experimental work in this field.

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