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Optical $\Gamma_6 \rightarrow \Gamma_8$ Free-to-Bound Transitions in Acceptor δ-Doped Single Heterostructure — Theoretical Analysis

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A theoretical analysis was carried out of an optical transition observed in high-quality GaAs/AlGaAs heterostructures δ-doped with shallow acceptors. The transition involves a 2D electron and a 3D acceptor-localized hole. The wave functions of a bulk Be acceptor were calculated within the spherical model with both the s-like and d-like parts of the envelope taken into account. The electron envelope wave functions resulted from self-consistent calculations of the electrostatic potential and were dependent on the 2D electron concentration, n_s. We show that: (i) including the d-like part of the acceptor envelope relaxes the selection rules of free-to-bound transitions at $k = 0$; (ii) in the magnetic field, the selection rules depend on the number of the electron Landau level; (iii) the ratio of the intensity of the strongest transitions in both circular polarizations is essentially different from 3:1, and strongly depends on n_s. These results show that a description that neglects the d-like part of the acceptor envelope is both qualitatively and quantitatively unjustified.

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1. Introduction

In acceptor δ-doped GaAs/AlGaAs heterostructures, a diluted sheet of shallow acceptors (typically Be or C) is introduced into GaAs some tens of nanometers from the GaAs/AlGaAs interface, and a two-dimensional electron gas (2DEG) is

created due to doping of a barrier with shallow donors. Because of a large separation of the δ-layer from the GaAs/AlGaAs interface, acceptors can be considered as embedded in a bulk GaAs. A photoluminescence experiment on such heterostructures reveals (among other features) a spectrum corresponding to the recombination of 2D electrons with holes localized in the δ-layer. An analysis of the degree of circular polarization (γ) of this free-to-bound $\Gamma_6 \to \Gamma_8$ transition in the magnetic field B allowed to investigate details of the electron–electron interaction and the spin polarization of 2DEG in the regime of the integer and fractional quantum Hall effects [1] and to investigate interaction of composite fermions [2]. The interest of Refs. [1] and [2] was focused on the investigation of 2DEG. It was assumed that properties of a hole localized on a shallow acceptor are known and properties of 2D electrons can be drawn from an analysis of the electron–hole luminescence. The hole was described as a quasi-particle with the envelope of an s-like character, and effects related to a non-zero wave vector of 2D electrons were neglected.

An opposite approach was proposed in Ref. [3]. The luminescence originating from the $\Gamma_6 \to \Gamma_8$ transition was analyzed at magnetic fields corresponding to even 2D electron filling factors which precisely sets to zero the spin polarization of the 2DEG. Then, the degree of polarization of the luminescence was determined by the polarization of acceptor-localized holes. In this way, since the polarization of 2DEG was defined, it was possible to investigate acceptor-localized holes. The main result of Ref. [3] was that at a constant magnetic field γ depends on the concentration of 2DEG, n_s, and that the observed dependence could be theoretically described if one takes into account (i) both s- and d-like parts of the acceptor envelope function; (ii) changes of 2D electron envelope functions with 2DEG concentration and the magnetic field; (iii) a proper set of selection rules of the $\Gamma_6 \to \Gamma_8$ free-to-bound transition, resulting from the presence of the d-like part of the envelope.

In a previous publication [3], we compared experimentally determined dependence $\gamma(n_s, B)$ with model calculations defined by the items (i)–(iii) listed above. The aim of the present paper is to describe in detail implications of the model adopted in interpretation of experimental data.

2. Comparison of the $L = 0$ and $L = 0, 2$ models

A simplified model description with the acceptor envelope approximated by the s-like part only will be called the $L = 0$ model, while that taking into account both $L = 0$ and $L = 2$ parts — the $L = 0, 2$ one. The $L = 0$ model is appropriate to describe a recombination of a free 2D electron with a free hole whose wave function is not modified by the electrostatic potential of the acceptor core. The selection rules corresponding to this case are shown in Fig. 1a.

Our goal here is to calculate matrix elements of optical transitions involving an electron in the first electrical subband and a hole localized on a Be acceptor

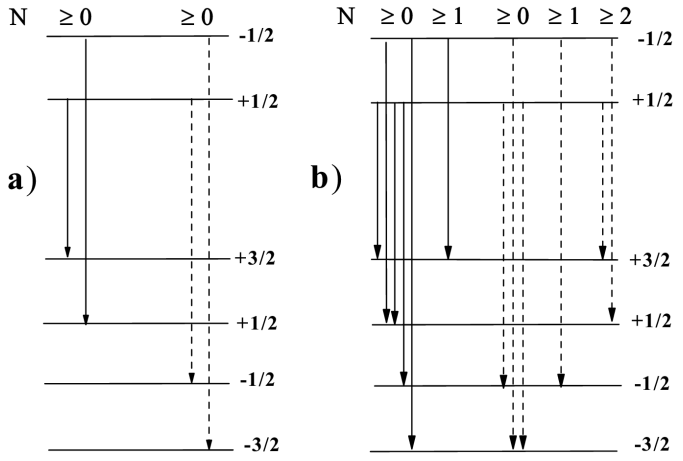

Fig. 1. Selection rules of $\Gamma_6 \to \Gamma_8$ free-to-bound transition according to (a) the $L = 0$ model and (b) the $L = 0, 2$ model at a nonzero magnetic field. Solid arrows: σ^- polarization; dashed arrows: σ^+ polarization. Electron levels are described with $j_z = \pm 1/2$; hole levels — with $F_z = \pm 3/2, \pm 1/2$. N is the number of the electron Landau level (after [3]).

situated at the distance z_0 from the GaAs/AlGaAs interface (in the calculations, $z_0 = 30$ nm, a typical distance in experimentally investigated structures [1–3]). Let us denote the electron envelope wave function as $c(z)\,\Psi(\boldsymbol{\rho})$, where $\boldsymbol{\rho}$ is the electron position in the xy plane where the 2DEG resides. $c(z)$ function results from self-consistent calculations of the electrostatic potential and depends on the electron concentration, n_s. In the case of zero magnetic field, $\Psi(\boldsymbol{\rho}) = \exp(\mathrm{i}\boldsymbol{k}\boldsymbol{\rho})$, where $\boldsymbol{k}$ is the electron wave vector in the xy plane. In the case of a non-zero magnetic field, $\Psi(\boldsymbol{\rho}) = \psi_{N,m}(\rho)$, where the functions $\psi_{N,m}(\rho)$ are analytical solutions of the Schrödinger equation in the symmetric gauge for the vector potential corresponding to the magnetic field $\boldsymbol{B} \| \hat{z}$. N is the Landau level number and $m\hbar$ is the z-th component of the angular momentum ($m \leq N$).

The Bloch part of the electron wave function, $u_{j=\frac{1}{2},j_z} = |R_0, \frac{1}{2}, j = \frac{1}{2}, j_z\rangle$ corresponds to the total angular momentum equal to $j = \frac{1}{2}$, and it is composed of s-like orbitals (denoted as R_0) and $\frac{1}{2}$ spinors. Thus, in the case $B = 0$ the electron functions are: $|\boldsymbol{k}, j_z\rangle = c(z)\exp(\mathrm{i}\boldsymbol{k}\boldsymbol{\rho})|R_0, \frac{1}{2}, \frac{1}{2}, j_z\rangle$. The calculations of matrix elements are easier to carry out with the envelope functions of the cylindrical symmetry. Let ϕ be the angle determined by the direction of the $\boldsymbol{k}$ vector in the xy plane. It is convenient to use the following superpositions of states $|\boldsymbol{k}, j_z\rangle$: $|\boldsymbol{k}, m, j_z\rangle = \frac{1}{\sqrt{2\pi}} \int \mathrm{e}^{\mathrm{i}m\phi}|\boldsymbol{k}, j_z\rangle \mathrm{d}\phi$. This cylindrical representation allows to use in the $B = 0$ case the same quantum numbers (m, j_z) as are used in $B \neq 0$ case.

The hole wave function is described within the spherical model of the acceptor [4]: $|\frac{3}{2}, F_z\rangle = f_0|L = 0, J = \frac{3}{2}, F = \frac{3}{2}, F_z\rangle + f_2|L = 2, J = \frac{3}{2}, F = \frac{3}{2}, F_z\rangle$,

where $f_0(r)$ and $f_2(r)$ are radial functions which are expressed as a sum of products of appropriate monomials and exponents, and are numerically calculated [4]. Functions $|L, J = \frac{3}{2}, F = \frac{3}{2}, F_z\rangle$ are superpositions of spherical harmonics Y_{LM} ($|M| \leq L$) and p-type Bloch functions $u_{J=\frac{3}{2},J_z} = |R_1, \frac{1}{2}, J = \frac{3}{2}, J_z\rangle$. The latter functions are, in turn, built with sp^3 orbitals R_1 and the spin $\frac{1}{2}$.

Even within the spherical approximation of the acceptor the whole symmetry of the system is not spherical but cylindrical in the both $B = 0$ and $B \neq 0$ cases. The selection rules depend on the Landau level number N and the matrix elements are nonzero for $m = F_z \pm 1 - j_z$, provided $|m| \leq 2$. Allowed transitions are shown in Fig. 1b and are compared to the case when the acceptor envelope function is described by the $L = 0$ model in Fig. 1a (here nonzero elements are for $F_z \pm 1 - j_z = 0$ only). In Fig. 1, the hole levels are described by F_z (which is equal to J_z in the case $L = 0$), and electron levels — by j_z. Figure 1 is plotted for $B \neq 0$. In the $B = 0$ case, all transitions indicated in Fig. 1 are allowed, but the Zeeman splitting of levels should be set to zero (no other transitions except these shown are allowed for $B = 0$).

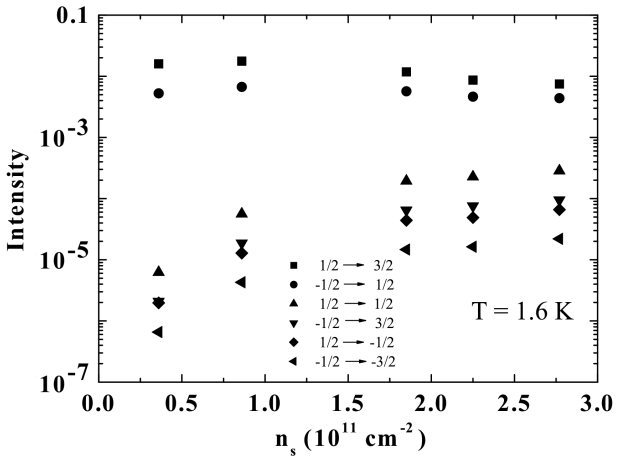

Fig. 2. Intensity of allowed transitions within the $L = 0, 2$ model for the σ^- polarization as a function of n_s.

Taking into account the $L = 2$ part of the acceptor envelope changes drastically selection rules of the transition considered. This makes an important qualitative difference between the two models. On the other hand, calculations of matrix elements of new allowed transitions show that their intensity is a few orders of magnitude smaller than that of transitions allowed within the $L = 0$ model. Figure 2 shows an example of these relations in the case of σ^- transitions. There is, however, much more important difference between the two models, shown in Fig. 3 for σ^- polarization, which is the ratio of the intensity of the two strongest transitions I_a: $1/2 \rightarrow 3/2$ and I_b: $-1/2 \rightarrow 1/2$ (the same is true for σ^+ transi-

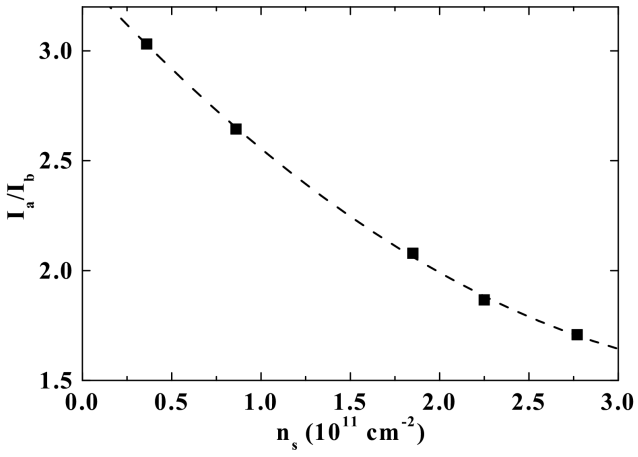

Fig. 3. The ratio of the strongest transitions for σ^- polarization, allowed both for the $L = 0$ and $L = 0, 2$ models, as a function of n_s.

tions, too). These transitions are allowed also within the $L = 0$ model. Within the $L = 0$ model, this ratio is equal to 3 by symmetry and does not depend on n_s. In the case of the $L = 0, 2$ model, the ratio shows a strong dependence on n_s, decreasing almost by a factor of 2 with n_s increasing from about zero to about 3×10^{11} cm^{-2}. This dependence influences calculated degree of polarization γ, and, for given magnetic field, makes γ calculated within the $L = 0, 2$ model quite different than that obtained within the $L = 0$.

3. Conclusions

In conclusion, we have shown that taking into account the d-like part of the acceptor bound hole changes qualitatively selection rules of the $\Gamma_6 \rightarrow \Gamma_8$ free-to--bound transition. Additional transitions become allowed, but their intensity is small. On the other hand, the ratio of transitions allowed also within the $L = 0$ model differs for $L = 0, 2$ and strongly depends on the 2DEG concentration which leads to a dependence of γ on n_s at a constant magnetic field, observed in Ref. [3].

Acknowledgments

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