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Optical and magneto optical responses assigned to probable processes of formation of exciton bound to an ionized donor in quantum dot

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ABSTRACT

The system formed by an electron and a hole coupled by Coulomb interactions with an ionized donor is the least known among the excitonic complexes. This complex is usually described as an exciton bound to an ionized donor. Strictly speaking, the exact mechanism of formation of this complex remains unclear. Two processes of formation giving rise to this system can be imagined. In a first process labeled A, the complex may be regarded as an exciton trapped by an ionized donor while in the second mechanism labeled B, this complex can be derived from the binding of a neutral donor and a hole. From a theoretical point of view both protocols can occur, with different probabilities and different binding energies, and consequently lead to different lines in the optical absorption spectra. In our hypothesis, we assume that the statistical mixture contains the two species coming from different origins and which were formed randomly. In this context of uncertainty and mixing processes, we propose to determine the absorption coefficient in the framework of the two possible hypotheses. In the aim to contribute with a valid description of the absorption spectrum, we report in this paper a full theoretical analysis of the optical and magneto-optical phenomena accompanying the two possible processes of formation, taking into account the dot sizes, the magnetic field strength, and the effect of the dielectric constant of the host material.

1. Introduction

The interest of quantum dots (QD) arise from their optical properties modulated by controlling their electronic characteristics through their sizes and shapes [1]. Manufacturers are able to accurately control the size of a QD and as a result they are able to "tune" the emitted light to a specific wavelength. Doping of these tiny objects not only offers more possibilities for tuning their electronic and optical properties but also diversifies their application spectra by inventing new optoelectronic devices [2,3]. In low dimensional structures, the enhancement of the Coulomb interactions between electron, hole and impurities, due to the geometrical confinement, leads to the stability of many excitonic complexes. With the progress achieved in optical spectroscopy, their experimental evidence are now unquestionable.

The optical transitions in confined system have been exhaustively investigated. In absorption or photoluminescence spectra, a large number of lines were observed, resulting from excitons bound to neutral or ionized impurities ((A^0,X), (D^0,X), (A^-,X) and (D^+,X)). Kozitsxii and Rack have calculated the generation of free and bound excitons by fast electrons within the framework of an extremely anisotropic model of a layer crystal finding that in the case of direct transition the oscillator strength of the exciton-impurity complex is two or three orders of magnitude higher than that for free excitons, whereas for indirect transitions this quantity greatly decreases with increasing distance between the extreme [4]. Benzaquen and coworkers have reported the temperature-dependent photoluminescence measurements to study the linewidth of the lower and upper polariton branches of the free-exciton transition in high-purity *n*-type InP epilayers with a concentration of neutral shallow donors [5]. Their study is a clear experimental evidence for the existence of: i) neutral shallow donor-bound-excitonic transitions, ii) combination of a neutral shallow donor to free-hole recombination with an ionized shallow-donor-bound-excitonic transition, iii) neutral deep-donor-bound-

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excitonic transition, and iv) neutral shallow-donor-acceptor pair recombination.

In low dimension semiconductors, very few experimental investigations show the existence of (D^+, X). We can cite the photoluminescence measurements performed in GaN epitaxial layers [6,7], where the authors identify these complexes by a line related to the recombination of excitons bound to ionized shallow donors. The transitions relative to a confined exciton and an exciton bound to an ionized donor or acceptor impurity located at the QD surface explain the origin of ultraviolet photoluminescence in ZnO quantum dots [8–10]. More recently Meyer et al. [11] showed that in ZnO heterostructures, the experimental localization energies fit linearly with the donor binding energies following the Haynes rule as $E(D^+,X) = 0.5\, E_{D^0} - 23.0$ (meV).

The transitions of these physical entities constitute a challenge to realize a new generation of optoelectronic quantum devices as single spin devices used in quantum information or single dopant transistor or in spintronic semiconductor devices such as memory chips by using magnetic QDs. Unfortunately, the theoretical investigation of these many body system is complicated. On the other hand, the problem most often encountered in spectral analysis is the fact that the lines of these systems are very close or superimposed which complicates the task to distinguish them. They are also sometimes masked by the line of exciton or neutral donor as in the case of the complex (D^+, X).

Indeed, one of the least known among these complexes is the system formed by electron, hole and an ionized donor (D^+, e, h) coupled by Coulomb interactions. This excitonic complex is described as an exciton bound to an ionized donor (D^+,X) but strictly speaking two processes of formation can give rise to this system. In a first process labeled A, the (D^+, X) complex may be regarded as an exciton trapped by an ionized donor [it means the binding between a correlated electron hole pair (e,h) and ionized donor, i.e. $(e,h) + D^+ \rightarrow (D^+, X)$] and in a second mechanism labeled B, the (D^+, X) can be derived from the binding of a neutral donor and a hole $(D^0 + h \rightarrow (D^+, X))$. From the theoretical point of view, these two protocols are possible with different probabilities and admit different binding energies and consequently lead to different lines in the optical absorption spectra. Unfortunately, no studies have been devoted to the optical absorption that accompanies the two processes. In our hypothesis, we assume that the statistical mixture contains the two species coming from different origins and which were formed randomly. Since each one of these species is formed according to the process A or B, they are therefore characterized by different optical responses.

In connection with this subject and in the aim to contribute with a valid description of the absorption spectrum, we report in this paper a full theoretical analysis of the optical and magneto-optical phenomena accompanying the two possible processes of formation of the (D^+, X) complex. We take into account the dot sizes, the magnetic field strength, and the effect of the dielectric constant of the host materials.

The paper is organized as follows: in section 2, we outline the theoretical framework of our approach based on the Elliott theory and using our own formalism [12] for determination of the different energies where the Schrödinger equation is solved numerically by means of variational method using a suitable wave function. In section 3 we discuss our numerical results and finally our conclusions are given in section 4.

2. Theory and method

In this section we present the main results of the theory of the electric dipolar absorption corresponding to a transition from an initial state $|i\rangle$ to a final state $|f\rangle$. We take into account the influence of an external uniform magnetic field. In confined systems the formalism for direct-gap semiconductors with parabolic bands at $k = 0$, is quite analogous to 2*D* or 3*D* cases [13]. For the sake of simplicity, we do not take into account all the details and possible degeneracies of the band structure, which we describe by an isotropic two-bands model. Because this theory is a natural extension of the well-known theory of the optical absorption of excitons [13–15], we present only its main results. Also, we do not take into account the influence of the temperature and restrict ourselves to one-photon transitions at 0 *K*.

In order to investigate the optical absorption coefficient (AC) relative to the (D^+,X) complex, we consider that the two different processes of transitions labeled A and B may occur as it has been mentioned in our introduction. In process A, the (D^+, X) complex may be regarded as an exciton trapped and disturbed by the existence of an ionized donor $(D^+ + (e,h))$ and admits as binding energy $E_b^A = E_e + E_h - E_{(D^+,X)}$. In the second process B, we consider that the (D^+, X) can be derived from the binding of a neutral donor and a hole $(D^0 + h)$ which corresponds to $E_b^B = E_{(D^+,X)} - E_{D^0} - E_h$. In this context of uncertainty and mixing processes, we propose to determine the AC in the framework of the two possible hypotheses.

We recall that the AC defined by Elliott between the initial $|i\rangle$ and final state $|f\rangle$ for an absorbed photon of energy $\hbar\,\omega$ is derived from the Fermi golden rule. It is given by the following relation [13–15]:

$$\alpha(\hbar\omega) = \frac{\pi e^2}{nc\varepsilon_0 m_0^2 \omega V} \sum_{i,f} \left| \left\langle f \left| \vec{\varepsilon} \cdot \vec{p} \right| i \right\rangle \right|^2 \delta\left(E_f - E_i - \hbar\omega\right). \tag{1}$$

Here n is the relative refractive index of semiconductor, c stands for the speed of light in vacuum, ε_0 is the dielectric constant of the vacuum, m_0 is the free electron mass, V the QD volume, and $\hbar\,\omega$ is the incident photon energy. $\vec{\varepsilon}$ is the light polarization vector and $\vec{p}$ is the momentum. The matrix element $\langle f|\vec{\varepsilon}\cdot\vec{p}|i\rangle$ depends deeply on the direction of the polarization and also governed by the strict selection rules. As established by several authors, when the incident light is assumed to be not-polarized the AC becomes [13–15]:

$$\alpha(\hbar\omega) = \frac{\pi e^2 E_p}{6nc\varepsilon_0 m_0 \omega V}\, I_{op}\, \delta\left(E_f - E_i - \hbar\omega\right), \tag{2}$$

where E_p is the well known Kane energy and I_{op} is the optical integral corresponding to the recombination of the electron and hole. It is given by Refs. [16–18]:

$$I_{op} = \left| \int \Psi\left(\vec{r_e}, \vec{r_h}\right) \delta\left(\vec{r_e} - \vec{r_h}\right) d\nu \right|^2. \tag{3}$$

The AC may then be simplified by approximating the δ function by a Lorentzian:

$$\delta\left(E_f - E_i - \hbar\omega\right) \approx \frac{\hbar\Gamma}{\pi\left[\left(E_f - E_i - \hbar\omega\right)^2 + (\hbar\Gamma)^2\right]}, \tag{4}$$

where $\hbar\,\Gamma$ is the maximum line width of the Lorentzian at mid-height [19]. Exact determination of the Lorentzian parameter Γ constitute a main problem in the determination of the optical AC and different values are used in the literature. Indeed, in absence of experimental data the Lorentzian parameter is usually taken such as $\hbar\,\Gamma$ is about ten times lower than the studied energy transition;

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