MAGNETO-ABSORPTION IN ELLIPSOIDAL QUANTUM DOT

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The absorption of light in ellipsoidal quantum dot in the presence of a magnetic field is discussed using perturbation theory. Also the same problem is discussed using the normal modes. Quantum dot absorption coefficient is calculated – as well as threshold frequency of absorption – as a function of applied magnetic field. Theoretical results are compared with experimental data obtained by magneto-luminescence method in $In_{0.53}Ga_{0.47}As$ quantum dot (M. Bayer et al, PRB vol.53, pp. 15810–15814, 1996).

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1. Introduction

The development of semiconductor technology has made possible the confinement of a finite number of electrons in a localized three-dimensional space of a few hundreds angstroms¹. This mesoscopic system, which was made up of artificially trapped electrons between a few layers of various semiconductors and called quantum dot (QD), opens new avenues in various technological applications. Almost all parameters of QDs: size, strength of a confining potential, number of electrons, coupling between dots, dielectric environment, the shape of tunneling barriers, as well as external parameters, such as temperature and magnetic, electrical and/or electro-magnetic fields, - can be varied in a controlled way². Therefore, QDs are often called “artificial atoms”. Modern nanotechnology allows to create and to study thoroughly physical properties of QDs with various geometrical shapes: spherical, cylindrical, ellipsoidal, pyramidal, etc^{3,4}.

Spherical and cylindrical QDs are most tractable objects, since for these sys-

tems one is able to construct realistic Hamiltonians that are analytically solvable at a strong confinement regime (noninteracting electrons or/and holes). In virtue of analytical solutions for eigenstates optical properties of such QDs can be studied thoroughly. One of the first attempts to analyse size quantization effects upon the interband optical transitions has been done in the model of infinitely high spherical well for different values of the QD radius⁵. This analysis was preceded by the optical absorption experiments for semiconductor balls embedded in a dielectric matrix⁶. The theoretical analysis demonstrated clearly that the blueshifting of the absorption onset is related with decreasing particle size. Interband transitions for cylindrical QDs were studied in^{7,8,9,10}. In cylindrical QDs one can vary two geometrical parameters (height and radius of the cylinder). It is well to bear in mind that the ideal spherical and cylindrical QDs are difficult to realize.

Optical properties of spheroidal QDs have been studied in^{11,12,13,14}. Recently the liquid phase epitaxy technique is used to create ellipsoidal QDs^{15,16}. The optical properties of such systems can be analysed with the aid of the model suggested in¹⁷, where the effect of the magnetic field on the QD spectrum has been studied. Evidently, that the variation of the magnetic field strength, along with the geometric parameters, enables to one to manipulate the QD energy spectrum more efficiently (see, for example,¹⁸ and references therein). In particular, due to the magnetic quantization, one can control the optical absorption edge in a QD.

The main focus of our paper is to develop a simple analytical model for analysis of interband optical transitions in ellipsoidal QDs in a homogenous magnetic field. To demonstrate the vitality of our model we will analyse the evolution of the interband transitions measured in magneto-luminescence investigations of $In_{0.53}Ga_{0.47}As/InP$ QDs¹⁹. The numerical results discussed below have been obtained for $In_{0.53}Ga_{0.47}As/InP$ QD ($\mu_e = 0.0463m_0$, $\mu_h = 0.61m_0$, $E_g = 0.75eV$, $\varepsilon = 10$).

2. Interband transitions in the absence of a magnetic field

In the effective mass approximation, we consider the QD confining potential in the following form:

$$V_{conf}(x, y, z) = \sum_{i=1}^3 \frac{\mu \omega_i^2 x_i^2}{2}, \quad (1)$$

where μ is the effective mass of an electron (hole), ω_i – confining frequency for a corresponding coordinate x_i . Confining frequencies, in general, for electron (hole) can be represented as follows

$$\omega_i^e = \frac{\gamma_i^e \hbar}{\mu_e l_i^2} \quad \left(\omega_i^h = \frac{\gamma_i^h \hbar}{\mu_h l_i^2} \right), \quad (2)$$

where γ_i^e (γ_i^h) – proportionality coefficients, characterizing the slope of the confining potential (in general they not equal to each other), l_i – values characterizing the confinement along the axes x , y and z .

The envelope wave function and energy spectrum of the electron (hole) can be written as:

$$\Psi(x, y, z) = \prod_{i=1}^3 C_{n_i} \exp\left(-\frac{x_i^2}{2a_i^2}\right) H_{n_i}\left(\frac{x_i}{a_i}\right), \quad (3)$$

$$E_{n_1, n_2, n_3} = \sum_{i=1}^3 \hbar\omega_i \left(n_i + \frac{1}{2}\right), \quad (4)$$

where $C_{n_i} = (2^{n_i} n_i! \sqrt{\pi} a_i)^{-1/2}$, $a_i = \sqrt{\frac{\hbar}{\mu\omega_i}}$.

In the dipole approximation, one is able to calculate the interband absorption coefficient in a strong quantization regime (see, for example,⁵):

$$K(\omega) = A \sum_{\nu_e, \nu_h} \left| \int \Psi_{\nu_e}^e \Psi_{\nu_h}^h dV \right|^2 \times \delta(\hbar\omega - E_g - E_{\nu_e}^e - E_{\nu_h}^h). \quad (5)$$

Here A is a coefficient proportional to the square of modulus of the dipole matrix element between Bloch functions; E_g is a bandgap width; $E_{\nu_e}^e$ ($E_{\nu_h}^h$) is an electron (hole) energy; ν_e (ν_h) is a set of quantum numbers characterizing the electron (hole) states; $\hbar\omega$ is a frequency of the incident light. The presence of delta-function ensures the energy conservation law for the corresponding transitions.

One obtains that the optical transitions occur only between levels of the same parity, i.e.

$$\begin{aligned} |n_1^e - n_1^h| &= 2t_1, \\ |n_2^e - n_2^h| &= 2t_2, \\ |n_3^e - n_3^h| &= 2t_3, \end{aligned} \quad (6)$$

where t_i – are integers.

For the threshold frequency, we obtain:

$$\begin{aligned} \hbar\omega_{00} &= E_g + E_0^e + E_0^h \\ &= E_g + \frac{\hbar}{2} \sum_{i=1}^3 (\omega_i^e + \omega_i^h). \end{aligned} \quad (7)$$

3. The effect of magnetic field on the interband transitions

Let us suppose that magnetic field B is applied on the system along the z axis. For a symmetric gauge

$$\vec{A} = 1/2[\vec{B} \times \vec{r}] \quad (8)$$

and at the condition $\text{div} \vec{A} = 0$, the QD Hamiltonian takes the following form

$$\begin{aligned} \hat{\mathcal{H}} &= \frac{1}{2\mu} \left[\hat{p} - \text{sgn}(e) \frac{e}{c} \hat{A}(\vec{r}) \right]^2 \\ &+ V_{conf}(x, y, z) = \hat{\mathcal{H}}_0 + \hat{\mathcal{H}}', \end{aligned} \quad (9)$$

where $\text{sgn}(e) = e/|e|$ defines the sign of the charge, $\hat{\mathcal{H}}_0 = \hat{p}^2/2\mu + \hat{V}(r)$ is the QD Hamiltonian in the absence of the magnetic field, and

$$\hat{\mathcal{H}}' = -\text{sgn}(e) \frac{e}{\mu c} \hat{\vec{A}} \hat{\vec{p}} + \frac{e^2 A^2}{2\mu c^2} \quad (10)$$

is the magnetic field contribution.

Let us consider first a weak magnetic field. At strong confinement regime, the impact of the magnetic field can be treated as a perturbation. In virtue of the gauge (8), the perturbation operator has the following form:

$$\hat{\mathcal{H}}' = \text{sgn}(e) i \hbar \omega_L \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right) + \frac{\mu \omega_L^2}{2} (x^2 + y^2), \quad (11)$$

where $\omega_L = eB/2\mu c$ is a Larmor frequency of the carrier.

The first order correction to the energy in the perturbation theory is determined by the diagonal elements of the perturbation operator $\hat{\mathcal{H}}'$ and is equal to:

$$\begin{aligned} E_{n_x, n_y, n_z}^{(1)} &= \langle n_x, n_y, n_z | \hat{\mathcal{H}}' | n_x, n_y, n_z \rangle \\ &= \frac{\hbar \omega_L^2}{4} \left(\frac{2n_x+1}{\omega_x} + \frac{2n_y+1}{\omega_y} \right), \end{aligned} \quad (12)$$

After some transformations one obtains

$$E_{0,0,0}^{(2)} = \frac{\hbar \omega_L^2}{4\omega_x \omega_y} \frac{(\omega_x - \omega_y)^2}{\omega_x + \omega_y} - \frac{\hbar \omega_L^4}{16\omega_x^3} - \frac{\hbar \omega_L^4}{16\omega_y^3}. \quad (13)$$

Collecting all results, we have for the ground state energy:

$$\begin{aligned} E_{0,0,0} &= \frac{\hbar}{2} \sum_{i=1}^3 \omega_i + \frac{\hbar \omega_L^2}{4} \left(\frac{1}{\omega_x} + \frac{1}{\omega_y} \right) \\ &+ \frac{\hbar \omega_L^2}{4\omega_x \omega_y} \frac{(\omega_x - \omega_y)^2}{\omega_x + \omega_y} - \frac{\hbar \omega_L^4}{16\omega_x^3} - \frac{\hbar \omega_L^4}{16\omega_y^3}. \end{aligned} \quad (14)$$

Fig. 1. Dependence of the semiconductor interband transition energy on the applied magnetic field B . Comparison of theoretical and experimental results (see¹⁹).

Before to calculate the interband optical absorption rate (5), a few remarks are in order. First, in general, the coefficients (γ) for an electron (γ_i^e) and a hole (γ_i^h) are not equal. The integral in (5) is nonzero only if n_z^h and n_z^e have the same parity. On the other hand, for two degrees of freedom (x and y) all transitions are allowed, while for z only transitions between states of equal parity are allowed (see (6)). Second, when the coefficients $\gamma_i^h = \gamma_i^e$, only the following transitions are allowed:

$$\begin{aligned} n_x^e - n_x^h &= 0, \pm 1, \pm 2; \\ n_y^e - n_y^h &= 0, \pm 1, \pm 2; \\ n_z^e - n_z^h &= 0. \end{aligned} \quad (15)$$

Finally, we obtain the threshold frequency of the absorption:

$$\hbar\omega_{0,0,0} = E_g + E_{0,0,0}^e + E_{0,0,0}^h. \quad (16)$$

Thus, the magnetic field removes the selection rules for the interband optical transitions in the ellipsoidal QDs, which hold for zero magnetic field. Due to the magnetic field not only transitions between electron and hole states of the same parity, but also between states of different parities can be implemented.

The evolution of the interband transition energies with the magnetic field is presented in Fig.1. The solid curve corresponds to our results, while the circles mark the experimental data¹⁹. The magnetic field increases the effective lateral confinement and, therefore, increases the energy level spacing. As a result, the interband transition energy for the ground state increases with the increase of the magnetic field.

4. Normal modes approach

For the gauge (8) the Hamiltonian (9) is a sum of two independent Hamiltonians

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_0 + \hat{\mathcal{H}}_z. \quad (17)$$

The Hamiltonian $\hat{\mathcal{H}}_z$ describes the dynamics in the z direction, which does not depend on the applied magnetic field

$$\hat{\mathcal{H}}_z = \frac{\hat{p}_z^2}{2\mu} + \frac{\mu\omega_z^2 z^2}{2}. \quad (18)$$

The Hamiltonian $\hat{\mathcal{H}}_0$ can be presented as follows¹⁸

$$\hat{\mathcal{H}}_0 = \frac{\hat{p}_x^2 + \hat{p}_y^2}{2\mu} + \frac{\mu}{2} \sum_{i=1}^2 \omega_i^2 x_i^2 - \omega_L \hat{l}_z, \quad (19)$$

where

$$\hat{l}_z = x\hat{p}_y - y\hat{p}_x \quad (20)$$

($\hat{l}_z$ is the z component of the angular momentum), and the following definitions are introduced:

$$\begin{aligned}\omega_1^2 &= \omega_x^2 + \omega_L^2, \\ \omega_2^2 &= \omega_y^2 + \omega_L^2.\end{aligned}\quad (21)$$

The eigenvalue problem for the Hamiltonian $\hat{\mathcal{H}}_0$ can be solved with the aid of the transformation from the coordinates x, y and the momenta $\hat{p}_x = m\hat{V}_x, \hat{p}_y = m\hat{V}_y$, to the normal modes $a_i^\dagger (a_i)$ ($i = \pm$)¹⁸

$$\begin{pmatrix} x \\ y \\ \hat{V}_x \\ \hat{V}_y \end{pmatrix} = \begin{pmatrix} X_+ & X_+^* & X_- & X_-^* \\ Y_+ & Y_+^* & Y_- & Y_-^* \\ V_x^+ & V_x^{+*} & V_x^- & V_x^{-*} \\ V_y^+ & V_y^{+*} & V_y^- & V_y^{-*} \end{pmatrix} \begin{pmatrix} \hat{a}_+ \\ \hat{a}_+^\dagger \\ \hat{a}_- \\ \hat{a}_-^\dagger \end{pmatrix}.\quad (22)$$

Here, $\hat{a}_i^\dagger (\hat{a}_i)$ is the creation (annihilation) operator of a new mode $i = \pm$ with commutation relations:

$$[\hat{a}_i, \hat{a}_j^\dagger] = \delta_{i,j}, \quad [\hat{a}_i, \hat{a}_j] = [\hat{a}_i^\dagger, \hat{a}_j^\dagger] = 0.\quad (23)$$

One can solve the equation of motion

$$[\hat{a}_i, \hat{\mathcal{H}}_0] = \hbar\Omega_i \hat{a}_i\quad (24)$$

and express the Hamiltonian $\hat{\mathcal{H}}_0$ by means of new normal modes

$$\hat{\mathcal{H}}_0 = \hbar\Omega_+ \left(\hat{a}_+^\dagger \hat{a}_+ + 1/2 \right) + \hbar\Omega_- \left(\hat{a}_-^\dagger \hat{a}_- + 1/2 \right),\quad (25)$$

where

$$\begin{aligned}\Omega_\pm^2 &= \frac{1}{2} (\omega_x^2 + \omega_y^2 + 4\omega_L^2) \pm \\ &\pm \frac{1}{2} \sqrt{(\omega_x^2 - \omega_y^2)^2 + 8\omega_L^2 (\omega_x^2 + \omega_y^2) + 16\omega_L^4}\end{aligned}\quad (26)$$

The solution of Eqs.(23),(24) enables to one to determine the coefficients of the transformation (22)

$$Y_\pm = iy_\pm, X_\pm = x_\pm,\quad (27)$$

$$x_\pm = 2\omega_L \frac{\Omega_\pm}{\Omega_\pm^2 - \omega_1^2 + \omega_L^2} y_\pm,\quad (28)$$

$$\begin{aligned}V_x^\pm &= -i\omega_L \frac{\Omega_\pm^2 + \omega_1^2 - \omega_L^2}{\Omega_\pm^2 - \omega_1^2 + \omega_L^2} y_\pm \\ &= -i\Omega_\pm \frac{\Omega_\pm^2 - \omega_2^2 - \omega_L^2}{\Omega_\pm^2 - \omega_2^2 + \omega_L^2} x_\pm\end{aligned}\quad (29)$$

$$\begin{aligned}
V_y^\pm &= \omega_\pm \frac{\Omega_\pm^2 - \omega_1^2 - \omega_L^2}{\Omega_\pm^2 - \omega_1^2 + \omega_L^2} y_\pm \\
&= \omega_L \frac{\Omega_\pm^2 + \omega_2^2 - \omega_L^2}{\Omega_\pm^2 - \omega_2^2 + \omega_L^2} x_\pm
\end{aligned} \tag{30}$$

$$y_\pm^2 = \pm \frac{\hbar}{2\mu\Omega_\pm} \frac{\Omega_\pm^2 - \omega_1^2 + \omega_L^2}{\Omega_+^2 - \Omega_-^2} \tag{31}$$

$$x_\pm^2 = \pm \frac{\hbar}{2\mu\Omega_\pm} \frac{\Omega_\pm^2 - \omega_2^2 + \omega_L^2}{\Omega_+^2 - \Omega_-^2}, \tag{32}$$

where $x_\pm$ and $y_\pm$ are real numbers.

Thus the electron (hole) energy spectrum in the ellipsoidal QD has the following form:

$$E = \hbar\omega_z(n_z + \frac{1}{2}) + \hbar\Omega_+ \left(n_+ + \frac{1}{2}\right) + \hbar\Omega_- \left(n_- + \frac{1}{2}\right). \tag{33}$$

The eigenstates of the Hamiltonian $\hat{\mathcal{H}}$ are

$$|n_+ n_- n_z\rangle = \frac{1}{\sqrt{n_+! n_-! n_z!}} (\hat{a}_+^+)^{n_+} (\hat{a}_-^+)^{n_-} (\hat{a}_{n_z}^+)^{n_z} |000\rangle. \tag{34}$$

Based on the obtained results the dependence of transition energy on the applied magnetic field, for any value of magnetic field strength, can be constructed. The mentioned dependence is represented on the Figure 2 for electron transitions between ground states of valence and conduction bands.

Fig. 2. Dependence of the semiconductor interband transition energy on the applied magnetic field B , without limitations on the value of magnetic field. Comparison of theoretical and experimental results¹⁹.

5. Summary

We propose a simple analytical model which can be useful for analysis of the interband optical transitions induced by a magnetic field. With the aid of this model we obtained a good description of experimental data reported in¹⁹.

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