Controlling Energy Spectra and Whispering Gallery Modes of Electrons in a Few Electrons Lateral QD

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Abstract. In this work, we study energy spectra and Whispering Gallery Modes (WGMs) of electrons in Quantum Dot (QD). It is shown that the WGMs can exist between two lowest energy levels of a QD, s- and p-states by taking into account the Coulomb interaction between the electrons in the QD, since in a few electron QD, Coulomb Interaction plays a crucial role in its energy spectrum. In literature, lateral QDs are usually modeled by a 2D harmonic oscillator. However, our calculations reveal that some degenerate energy levels would be created due to the height of the QD. The effect of the dimension of the QD, and magnetic field are also investigated on the energy spectra.

1. Introduction

Semiconductor Quantum Dot (QD) can be considered as an artificial atom, and reveal discrete energy levels. By measuring current versus gate voltage of a QD, Ref. [1], shows that it has similar properties of atoms, as filling the shell structures in a 2D harmonic oscillator. Using high-resolution capacitance spectroscopy, Ref. [2] shows that energy levels of InAs QD are similar to s-, p- and d-shells. In order to model interband spectroscopy, in Ref. [3], Coulomb interaction between electrons and also electrons and holes are calculated and treated as a perturbation, where confining potential is considered to be parabolic and two-dimensional. Using high spatial resolution optical spectroscopy, [4] studies structural and optical properties of InP/GaInP QDs, while in [5] WGMs are depicted in these dots which can be in the resonance of Wigner Molecules (WMs) (crystallization of electrons in a confined structure with a few amounts of electrons).

Regarding some anomalies in radiation spectra and intermixing of energy levels of the QDs, this paper studies QDs with another point of view and tries to consider the major phenomena that can affect its energy spectra. It shows that the dimension of the QD including its height has a critical effect on the QD’s energy spectra. The Coulomb interaction is comparable to the energy of interband transition which can cause intermixing energy bands even for zero magnetic field.

2. Energy Spectra

The Schrödinger equation is solved in cylinder coordinate for a InP lateral QD embedded in GaAs substrate, and it is treated as a partial differential equation (PDE). Therefore, in Comsol Software, a coefficient form PDE is defined, for each of the QD and substrate, and its eigenvalues...
Figure 1. Energy spectra of QD with (a) 4 meV and (b) 2 meV energy splitting.

Figure 2. Wavefunctions of QD for $m = 0$: 3rd (top-left), 4th (top-right), 5th (bottom-left), 6th (bottom-right) eigenfunctions.

and eigenfunctions are calculated numerically [6]. Figure 1(a) shows energy spectrum of a QD for which its dimensions (length: 114 nm and height: 14 nm) is adjusted in order to achieve 4 meV energy splitting between two lowest energy levels, $s$ and $p$. This figure shows some energy degeneracies for each azimuthal number ($m$). The wavefunctions of the QD (Fig. 2) shows that these degeneracies are due to the changing the quantum number associated to the height of the QD ($z$-direction). It starts between 5th and 6th eigenvalues and the splitting increases with increasing azimuthal number.

Figure 1(b) shows that with changing the dimension of the QD (length: 150 nm and height: 26 nm), one can manipulate its energy spectra. In fact, smaller splitting between two lowest energy levels, $s$- and $p$-states, leads to the denser energy spectra, and it is more likely that energy
2.1. Coulomb Interaction

Direct and exchange Coulomb interaction between two wavefunctions can be calculated from Eqs. (1) and (2), respectively:

\[ V_d = \frac{e^2}{4\pi \varepsilon_0 \varepsilon_r} \int \int \frac{\psi_1(r_1)^2 \psi_2(r_2)^2}{r_{12}} dv_1 dv_2 \]  

(1)

\[ V_e = \frac{e^2}{4\pi \varepsilon_0 \varepsilon_r} \int \int \psi_1^*(r_1)\psi_2^*(r_2)\psi_1(r_2)\psi_2(r_1) \frac{1}{r_{12}} dv_1 dv_2 \]  

(2)

We assume a QD which contain 5 electrons and also one electron in the excited state. Figure 3(a) shows two different arrangement of the electrons, one with a excited electron in p-state (top) and another in WGM-state (bottom).

In Fig. 3(a) (top), coulomb energy of one of the electron in \( p_x \) orbital is

\[ C_1 = [p_xp_x] + [2p_xp_y - (p_xp_y)] + [2sp_x - (sp_x)] \]  

(3)

where exchange coulomb interaction are shown with index e. In Fig. 3(a) (bottom), coulomb energy of the electron in \( wgm_x \) is

\[ C_2 = [p_xwgm_x - (p_xwgm_x)] + [2p_ywgm_x - (p_ywgm_x)] + [2swgm_x - (swgm_x)] \]  

(4)

The calculated Coulomb energy difference between these two arrangements in Fig. 3(a) is \( C_1 - C_2 = 5.93 \text{ meV} \). Therefore, if we assume s and p states of the QD, same as their single particle energy levels, \( wgm \) with \( m = 2 \) would be decreased by 5.93 meV.

Figure 3(b) shows energy spectrum of the QD with taking into account the Coulomb interaction where we assume the first eigenstates of azimuthal number \( m = 2, 3, \ldots \) as \( wgm \), the second eigenstates of \( m = 0, 1, 2, \ldots \) as \( XII \), and third eigenstates of \( m = 0, 1, 2, \ldots \) as \( XIII \). This figure shows \( wgm \) state with \( m = 2 \) between s- and p-states.

Figure 3. (a) Two different arrangements of electrons. (b) Energy spectra by considering Coulomb interactions.

levels intersect each other, due to the Coulomb interaction, magnetic field, etc.
2.2. Magnetic Field

Figure 4 shows eigenergies of QD for 4.1 meV s-p states splitting, where quantum numbers \((n, l)\) related to the radial and azimuthal number are specified for each of the levels.

To make our system equivalent to the 2D harmonic oscillator energy levels, a detuning parameter \(\Delta_{n,l}\) is introduced in the 2D harmonic energy levels as:

\[
E_{n,l} = (2n + |l| + 1)(\hbar\omega_0 + \Delta_{n,l})
\]

For each energy level, the detuning parameter can be determined in order to make it equivalent to its 2D harmonic energy level. On the other hand, energy levels of a 2D harmonic oscillator with applying magnetic field can be calculated from:

\[
E_{n,l} = (2n + |l| + 1)\sqrt{\frac{1}{4}(\hbar\omega_c)^2 + (\hbar\omega_0 + \Delta_{n,l})^2} - \frac{1}{2}l\hbar\omega_c ; \quad \hbar\omega_c = \frac{\hbar eB}{m^*}
\]

where \(\omega_c\) is cyclotron frequency. With magnetic field \(B = 1\ T\) it is calculated that energy level of s-state would be increased by 0.0634 meV, p-state with \(l = -1\) would be increased by 0.8503 meV and wgm state with \(l = 2\) would be decreased by 1.2619 meV.

3. Conclusion

It shows that lateral QD cannot be considered as a pure 2D dimensional harmonic oscillator, and its dimension including height, has a major effect on its energy level and transition band. Therefore, Schrodinger equation is solved for a 3D QD, in cylinder coordinate, numerically. It shows that Coulomb interaction is comparable or higher than interband transition which leads to intermixing of the energy levels. The effect of the magnetic field is also investigated.

References

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