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Stark-shift of impurity fundamental state in a lens shaped quantum dot

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ABSTRACT

We calculate the Stark effect and the polarisability of shallow-donor impurity located in the centre of lens shaped quantum dot by a variational method and in the effective-mass approximation. Our theoretical model assumes an infinite confinement to describe the barriers at the dot boundaries and the electric field is considered to be applied in the *z*-direction. The systematic theoretical investigation contains results with the quantum dot size and the strength of the external field. Our calculations reveal that the interval wherein the polarisability varies depends strongly on the dot size.

1. Introduction

Recent advances in the fabrication techniques of nano-meter sized structure of crystals have been arousing considerable interest. Especially low-dimensional semiconductor structures have been extensively investigated both theoretically and experimentally. During the growth process it is possible, intentionally or unintentionally, to add impurities into the nano dot [1]. So an understanding of the nature of impurity states in semiconductor structures is one of the crucial problems in semiconductor physics because impurities can dramatically alter the properties and performance of the quantum devices [2]. The incorporation of impurities into a quantum dot (QD) affects considerably the optical and transport properties and can explain the new photo-luminescent transition in optoelectronic devices [3]. From theoretical side, this poses a class of eigenvalue problems in a coulombic potential with specific boundary conditions. In some cases the problem is solved and the simplest model is the case of an impurity located in the centre of spherical QD. However the spherical cavity is still not good enough for a real QD [4]. In many cases pyramids, truncated pyramids or lenses provide better spatial descriptions of the QD geometries than spheres, ellipsoids or even parallelepipeds [5]. In a self-organised growth process one often finds lens-shaped QDs with cylindrical symmetry around the growth direction [6]. Indeed the Schrödinger equation itself is unchanged but the boundary conditions imposed by the geometry have an important impact on the theoretical solutions. That is, in the QD systems the additional quantum confinement dramatically changes the optical and electronic properties, compared to those in bulk structures [7,8]. An external control of the QD properties can be achieved quite straightforward. This includes the manipulation of the QD eigenstates in a well-defined manner by applying external electric or magnetic fields [9]. The existence of the external quantising fields often results in restructure of the energy levels, as well as creation of new selection rules in the process of the light absorption [10].

The phenomenon of the change in the optical properties of semiconductor nanostructures in response to an electric field manifests itself in spectral shifts and changes in the intensities of the absorption maxima [11]. Moreover semiconductor optoelectronic modulators based on the quantum-confined Stark effect (QCSE) are attractive transmitters to convert signals from the electronic into the optical domain and vice versa [12]. So understanding the QCSE is important from both fundamental physics and device applications perspectives. That is why lot of works have been devoted to the study of the Stark effect in semiconductor nanostructures [11,13–15]. In this context Chen-Kai Kao et al. [16] studied the performance of UV electro absorption modulators based on bulk GaN films and GaN/AlGaN multiple quantum wells and they found that the absorption can be strongly modified through the application of an external electric field. Achtstein et al. [11] also performed a study on electro absorption in CdSe colloidal QDs, nanorods, and nanoplatelets exposed to an electric field. They concluded that the experimental findings require an elaborate theory of electro absorption which should take into account different responses of the electronic systems, of the structures, to the external electric field. From the side of the theoretical studies, they usually focuses on the study of one particle (electron or hole) or an exciton. Wang et al. studied the transverse Stark effect of electrons in semiconducting quantum boxes and they concluded that the large Stark shift leads to an obvious reduction of the inter band recombination and wide irradiance spectrum [8].

Terzis and Baskoutas [17] investigated the effect of electric and

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magnetic field on the binding energy of a donor states in GaAS QD, they found that the binding energy decreases as the electric field increases. Morales et al. [18] included the effect of the hydrostatic pressure in their study; their conclusion was that the impurity binding energy and polarisability can be tuned by means of an applied external electric field or hydrostatic pressure. They added that this behaviour could be used in the design and construction of semiconductor devices.

Elsewhere, the polarisability determines the sensitivity of the exciton energy to an electric field. Moreover, for applications of QDs as emitters and detectors, the polarisability should be large so that the energy can be tuned over a large range with modest electric fields [19]. An example of a lens-shaped geometry may be found for InAs QDs grown on InP [20] and they can be well described by the geometry imposed by the parabolic coordinates [5]. To our knowledge there is no study concerning the effect of an electric field on an impurity located in the centre of such a geometry.

The aim of this work is to present a variational calculation of the shift of the energies for a hydrogenic impurity located in the centre of a symmetrical paraboloidal quantum dot (SPQD) and submitted to an external electric field using an infinite hard-wall confining potential. This particular potential avoids the existence of quasi bound states for strong fields, since a strong enough electric field combined with finite confining potential will tend to eject the carrier (the electron) from the bound state. The dependence of the polarisability on the applied electric field and the size of the SPQD is also studied and discussed.

2. Theoretical framework

We consider an impurity donor confined in the centre of a SPQD (see Fig. 1). The electric field is applied along the z-axis.

In order to describe the interplay between the spatial confinement of the electron which is due to the geometry of the QD, the external electric field, and the attractive Coulomb interaction between the electron and the donor, which is in the centre of the geometry, we use the following Hamiltonian in effective mass approximation and neglecting the band-structure effects:

$$H = -\frac{\hbar^2}{2m_e^*}\nabla^2 - \frac{e^2}{\kappa r} + eFz + V_w, \tag{1}$$

where m_e^* and e are the electron effective mass and its charge respectively, κ is the static dielectric constant, F is the electric field which is applied in the z-direction, and r is the distance of the electron from the impurity site (see Fig. 1). V_w is the confining potential which vanishes inside the dot and becomes infinite outside. The assumption of a constant electric field is justified by a negligible difference between the dielectric constants of the dot and its surroundings.

Using the effective Rydberg constant $R_y = \hbar^2/2\, m_e^*\, a^{*2}$ as the unit of

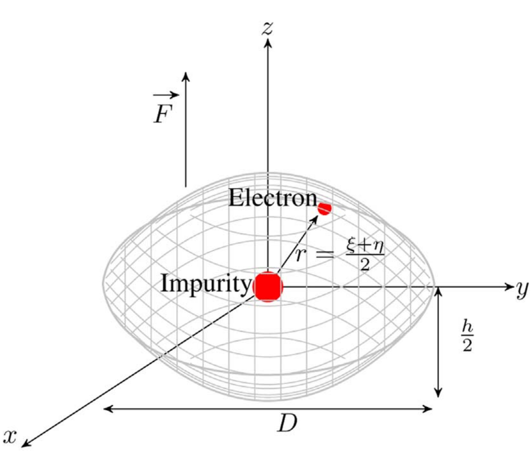

Fig. 1. The symmetrical paraboloidal quantum dot (SPQD) geometry is characterised by the thickness at the centre h, the circumference diameter D, and the volume $V = \frac{\pi}{8}hD^2$.

the energy, the effective Bohr radius $a^* = \kappa\, \hbar^2/m_e^*\, e^2$ as the unit of the length, and $F_0 = e/\kappa\, a^{*2}$ as unit of the electric field intensity the Schrödinger equation reads:

$$H = -\nabla^2 - \frac{2}{r} + 2fz. \tag{2}$$

Here $f = \frac{F}{F_0}$ is the dimensionless measure of the electric field. We recall that F_0 is twice the donor ionisation defined by Blossey [21].

Owing to the geometry of the lens shape considered in this work, it is more suitable to use the parabolic coordinates system (ξ, η, φ) related to the Cartesian coordinates by [22]:

$$x = \sqrt{\xi\eta}\cos\varphi,$$
$$y = \sqrt{\xi\eta}\sin\varphi \tag{3}$$
$$z = \frac{1}{2}(\xi - \eta),$$

with $0 \le \xi < \infty$, $0 \le \eta < \infty$, and $0 \le \varphi \le 2\pi$. This coordinate system has been used in the literature for example by to study the hydrogen atom [23–25], and to study the paraboloidal QD [4,26,5,27]. In this coordinate system the Hamiltonian takes the following form:

$$H = -\left\{\frac{4}{\xi+\eta}\left[\frac{\partial}{\partial\xi}\left(\xi\frac{\partial}{\partial\xi}\right) + \frac{\partial}{\partial\eta}\left(\eta\frac{\partial}{\partial\eta}\right)\right] + \frac{1}{\xi\,\eta}\frac{\partial^2}{\partial\varphi^2}\right\} - \frac{4}{\xi+\eta} + f(\xi-\eta). \tag{4}$$

The impurity energy in the presence of electric field is calculated by the traditional variational method which consist of choosing a trial ground state wave function, calculating the corresponding energy and minimising it. In the absence of the electric field (f=0) the variables in the Hamiltonian in Eq. (4) are separable. When the electric field is considered ($f \neq 0$), the Hamiltonian separates partially [28] and under such conditions several alternative methods (for instance, diagonalisation with appropriate basis, finite elements method, finite differences methods, and variational method) can be used to find the eigenvalues and eigenfunctions of the differential equation. Assaid et al. [26] have studied a donor impurity located at the centre of a SPQD. For the bound state the solution is given by

$$\Psi_0(\xi,\eta,\varphi) = N\exp\left(-\frac{\xi+\eta}{2\Omega}\right)\left(\frac{\xi\eta}{\Omega}\right)^{|m|/2} \times M\left(\frac{1}{2}+\frac{|m|}{2}-\beta\Omega,\, 1+|m|,\, \frac{\xi}{\Omega}\right)M\left(\frac{1}{2}+\frac{|m|}{2}-\gamma\Omega,\, 1+|m|,\, \frac{\eta}{\Omega}\right), \tag{5}$$

where $\Omega = \sqrt{\frac{-1}{2E}}$ (note that for the bound state E is negative [26]), N is the normalisation constant, and M denotes the Kummer's confluent hypergeometric function. β and γ are two arbitrary separation constants except for the constraint $\beta + \gamma = 1$. The ground state wave function correspond to $\beta = \gamma = 1/2$. The application of an external electric field leads to a distortion of the symmetry and polarises the orbitals in the electric field direction. Here we follow the work by Duque et al. [29] and we choose as a variational function the product between the impurity-related wave function in Eq. (5) and a z-dependent exponential function which takes into account the electric field effects. In this work, the maximum value of the applied electric field will be 300 kV/cm and consequently only the first two terms of the Taylor's series of the exponential function will be necessary to describe the electric field effects. Such approximate trial wave function has been previously used in the literature for donor impurities and excitons in QD under static applied electric field [30–32]. So in this conditions the hydrogenic problem for the Hamiltonian in Eq. (4) may be solved by choosing the impurity ground state trial wave function as

$$\Psi(\xi,\eta,\varphi) = \Psi_0(\xi,\eta,\varphi)(1 + \alpha f(\xi-\eta)), \tag{6}$$

where α is a variational parameter. The resulting equation to solve reads

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