Binding energy of donor states in a GaAs quantum dot: Effect of electric and magnetic field

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Abstract. Using the potential morphing method, the effects of electric or magnetic field on the binding energy of the hydrogenic impurity in disc-like GaAs quantum dots with parabolic confinement have been studied in details. Our results indicate that the binding energy of impurities decreases as the electric field increases. Moreover the relative reduction of the binding energy decreases as the strength of the confining potential decreases. Finally the magnetic field investigations have shown that the binding energy increases as the applied magnetic field increases.

1. Introduction

Recent advances in microfabrication technology have allowed the construction of structures with lower dimensions. The most recent achievement is the fabrication of zero dimension quantum structures, usually called quantum dots. Due to their small size these structures present physical properties that are quite different from those of the bulk semiconductor constituents [1,2]. It is expected that these properties will exhibit more pronounced differences as the confinement is increased with the lowering of the dimensionality. More specifically, the shape and the size of the nanostructure have a strong influence on the optical properties [3].

Due to the fact that impurities in semiconductors influence both transport and optical properties, topics like confined donors or acceptors in quantum dots have been extensively investigated [4-10]. The understanding of the nature of the impurity states in semiconductor structures is one of the crucial problems in semiconductor physics. Impurities can alter the properties and performance of a low dimensional structures operating in the quantum regime, which are usually very sensitive to variations in composition and geometry. Several numerical methods have been developed in order to systematically investigate the physical properties of the impurity embedded in a quantum dot. Most known is the variational method [11-18], a technique where a trial wave function should be guessed. Other method include tight binding self consistent linear screening technique [19] the strong confinement approach [20,21] and the perturbation approach [8,18].

In a recent publication of our group [22], using the potential morphing method [23,24], we have verified the strong dependence of the donor binding energies on the dot size/shape and the impurity position within two- and three-dimensional GaAs quantum dots. In the present work the influence of the
electric and magnetic field for on- and off-center hydrogenic impurities within two-dimensional disk-like quantum dots, will be systematically investigated and will be compared to existing theoretical results.

2. Electric field effects on the binding energy
In this section we investigate the electric field effect on the binding energy of hydrogenic impurities in quantum dots with parabolic confinement using the potential morphing method. The results are compared to existing studies where variational approaches have been used [25-27].

The Hamiltonian of the system is given by the expression

$$H = \frac{p^2}{2m^*} + \frac{1}{2} m^* \omega^2 \mathbf{r}^2 - \frac{e^2}{\varepsilon |\mathbf{r} - \mathbf{r}_i|} + \mathbf{E} \cdot (\mathbf{r} - \mathbf{r}_i)$$

(1)

where $m^*$ is the electron effective mass, $e$ the electronic charge and $\varepsilon$ is the dielectric constant of the dot material, $\mathbf{r} = (x, y)$ is the position vector of the electron, $\mathbf{r}_i = (x_i, y_i)$ is the position vector of the fixed hydrogenic impurity and $\mathbf{E} (= E \hat{\mathbf{z}})$ is the external applied electric field.

The binding energy is generally defined as the difference between the ground state energies of the above Hamiltonian with and without the Coulomb term, respectively. The impurity can be in any position within the quantum dot. In order to be consistent with previous investigation by Lien and Trinh [25], effective atomic units are used. Therefore, all energies are measured in units of the effective Rydberg \( R^* \equiv m^* e^4 / 2\hbar^2 e^2 \), all lengths are presented in units of the effective Bohr radius \( a_B^* \equiv \hbar^2 e / m^* e^2 \) and the confinement potential being \( m^* \omega^2 r^2 / 2 = \beta^2 r^2 \). As the dot radius is inversely proportional to \( \beta \), the usage of the bulk parameters in the nanoscaled structures is a common practice in most theoretical investigations [25].

We concentrate exclusively on the ground state. Figure 1(a) shows the binding energy, measured in units of the effective Rydberg energy, as a function of the effective field \( F \equiv E / 2\beta^{1/2} \), as the measure of the electric field \( E \) for a given value of \( \beta \) (i.e. given dot radius). Taking GaAs as a typical quantum dot material, we use the bulk values [28]. Hence, one has \( m^* = 0.067 m_e \) (electron effective mass) \( \varepsilon = 12.9 \) (dielectric constant), \( a_B = 10.19 \)nm (Borh radius), and therefore \( R^* = 5.478 \)meV [28]. The usage of the bulk parameters in the nanoscaled structures is a common practice in most theoretical investigations [25].

In figure 1(a), the position of the donor impurity is at the center of the disk like quantum dot. Our findings are in excellent agreement with those reported by Van Lien and Trinh in ref. 25. In figure 1(b), we estimate and depict the binding energy for an impurity position at distance equal to half the quantum dot radius. We clearly observe a very similar behavior as in figure 1(a), but all binding energies are reduced as it is expected (almost by the same factor, independently of the \( F \) value).

3. Magnetic field effects on the binding energy
In this section we study the magnetic field effect on the binding energy of hydrogen impurities in quantum dots. The effect of an external magnetic field on the energy spectrum is one of the very powerful tools for the study of the electronic states of the quantum dots.

The magnetic field effects on the related optical transitions have been studied extensively for impurities in bulk semiconductors [29]. Although the magnetic field effects on the conduction electron energy levels have been studied extensively [30,31], there are very few investigations on the semiconductor systems of low dimensions [32].
The binding energy, measured in units of the effective Rydberg energy, as a function of the effective field $F$ for quantum dots with $\beta =1, 0.5, 0.25$ and $0.1$. The value of the effective field $F=1$ corresponds to an applied electric field of $5.4\times10^5$ V/m for $\beta =1$ and to a field of $3\times10^4$ V/m for $\beta =0.1$. The position of the donor impurity is at (a) the center of the quantum dot and (b) at $r=0.5R$.

The effective mass Hamiltonian of a system consisting of an electron bound to a donor impurity, inside a disk-like quantum dot of radius $R\equiv\left(h/(m^{*}\omega)^{1/2}\right)$, with a confining potential, in an external magnetic field $B(=B\hat{z})$ has the form

$$H = \frac{1}{2m^{*}}(p - \frac{e}{c}\vec{A})^2 + \frac{1}{2}m^{*}\omega^2 r^2 - \frac{e^2}{\varepsilon|\vec{r} - \vec{r}_d|}$$

where $\vec{A}$ is the vector potential of the magnetic field $\vec{B}$. For a uniform magnetic field we can be written $\vec{A}(r) = \frac{1}{2}\vec{B}\times\vec{r}$. The magnetic field is assumed to point along the z-axis, i.e. its direction is perpendicular to the disk plane.

In figure 2(a) and 2(b) the binding energy is plotted as a function of the applied magnetic field for two different values of the quantum dot radius. It is clearly observed that the donor binding energy is increasing as the applied magnetic field increases. This behaviour is almost linear in the region of weak magnetic fields ($B < 10T$).
4. Conclusions
In conclusion, the binding energy of hydrogen impurities in quantum dots with parabolic confinement decreases as the electric field increases and the relative reduction gets smaller with decreasing strength of the confining potential and increases as the applied magnetic field increases.

5. References
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