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1s-like state binding energy of a donor impurity bound to Xz valleys of GaAs/AlAs type II quantum dots with an uniform applied magnetic field

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Abstract. In this paper we calculate the binding energy of a donor impurity in the 1s-like state bound to X valleys of GaAs/AlAs type II quantum dots, using an anisotropic variational method, which allows us to take into account the anisotropy of the effective mass and quantum confinement. The binding energy is plotted against the radius of the cylinder and the uniform magnetic field applied along the cylinder axis. The binding energies have a monotone behavior with the cylinder radius for different magnetic fields and almost constant behavior with increasing magnetic field.

1. Introduction

The The study of low dimensional heterostructures type II has increased in recent years especially for potential applications such as infrared detectors[1], devices for use in spintronics[2], and including the observation of the called Aharonov-Bohm effect[3] and it is also use for creating a laser device in the infrared[4] and green[5]. Also it has been observed phononic effects in type II superlattices that would allow the development of sound amplification devices by stimulated emission[6]. The study of type II quantum dots has been expanded in recent years. Najjar et al.[7], studied the exciton recombination in quantum dots and wells of ZnTe/ZnSe. Kai Cui et al.,[8] observed emission spectrum of multilayer self-assembled quantum dots GaSb/GaAs at room temperature. Dag Wang et al.,[9] studied the binding energy of the ground state of shallow donor impurities in type II materials depending on the width of the well, considering mixing the Γ and X valleys in a structure of AlAs/GaAs, which leads to a differences in the behavior of the energy compared with type I. Carneiro and Weber[10] calculated the energy of the ground state and some excited states for donor impurities in the X valley of a type II quantum wells, they obtained a strong dependence of the binding energy with the effective mass of the carriers and the symmetry of the valley. Gulyaev et al.,[11] studied the recombination of carriers in a type II superlattice doped with acceptor and donor impurities through photoluminescence, and they found that the increase in the binding energy of the impurities results in a decrease in the rate of recombination.

In this paper we report the calculation of the binding energy for a donor impurity centered in a type II quantum dot of AlAs/GaAs, with cylindrical geometry and an applied magnetic field. We study the energy behavior in function of geometrical parameters of the dot and the magnetic field variation.

2. Theoretical Model

We consider a heterostructure based on two concentric cylinders, the inner radius R and height L correspond to the AlAs cylindrical structure, the outer radius R + a and height $L + 2a$ correspond to the GaAs cylindrical

structure and they are located within a matrix of $Ga_{1-x}Al_xAs$, the magnetic field (B) is applied in the direction of the cylinders axis, as shown in Figure 1

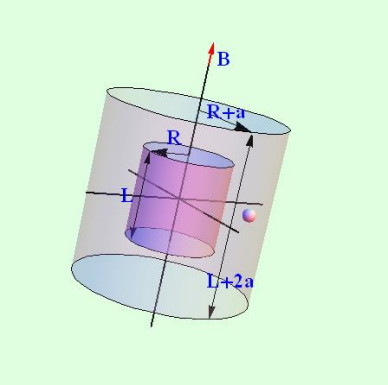

Figure 1. Heterostructure scheme of a type II quantum dot with a donor impurity in (sphere) and a uniform magnetic field applied, the inner cylinder is considered AlAs, the outward is GaAs, and the entire system is within a matrix of $Ga_{1-x}Al_xAs$.

We used a Hamiltonian in cylindrical coordinates (ρ,φ,z) given by

$$H = \frac{1}{2}(P_i - eA_i)m_{ij}^{-1}\left(P_j - eA_j\right) + V_{eff}(r) \quad (1)$$

Where P_i is the momentum operator, A_i is the vector potential, associated with the magnetic field (B), m_{ij} is the effective mass tensor, i,j run over ρ,φ,z coordinates, and V_{eff} is the effective potential due to coulomb and geometrical confinement potential. The last one is given by

$$V(\rho) = \begin{cases} V_0\left(\frac{\rho}{R}\right)^2, & \rho < R \\ V_0, & R \le \rho < R + a \\ V_1, & \rho \ge R + a \end{cases}, \quad V(z) = \begin{cases} 0, & 0 \le z \le L \\ V_0, & 0 > z > -a, \ \wedge, \ L < z \le L + a \\ V_1, & z < -a \wedge z > L + a \end{cases} \quad (2)$$

The coulomb interaction, in arbitrary units, is $V = -\frac{2\tau}{|\vec{r}-\vec{r}_{imp}|}$.When the coulomb interaction is not considered (τ=0) in V_{eff} the Schrödinger equation, for an electron in the structure, have analytic solution given by ψ_0 and its energy is E_0. When the coulomb interaction is taking in account (τ=1) in V_{eff} the Schrödinger equation ($H\psi=E\psi$) is solved by a variational method. We considered a Bastard[12] type function given by

$$\Psi(\rho, z, \phi) = \Psi_0 Exp\left(-\sqrt{\frac{(\vec{\rho}-\vec{\rho}_i)^2}{\lambda_1^2} + \frac{(z-z_i)^2}{\lambda_2^2}}\right) \quad (3)$$

where λ_1 y λ_2 are variational parameters, $\vec{\rho}_i$ and z_i, are the impurity position along the perpendicular and parallel direction to the magnetic field. We calculated the binding energy, E_b=E_0-E, as a function of the geometrical parameters and the magnetic field, $\vec{B} = B\hat{k}$, symmetric gauge for the potential vector is considered.

3. Results and Analysis

In the numerical calculations it has been used the following parameters for AlAs material, dielectric constant ε = 10.06, well barrier height 316 meV., alignment of the conduction bands and valence in 35% and 65%, respectively. From the bottom of the Γ conduction band, in the GaAs, to the bottom of the X valley, in the AlAs, there is a difference of 145 meV. The values of the effective mass in the equation 1 depend on the X valley under consideration. The two sets of effective masses in volume of AlAs ($m^*_\perp = m^*_{x,\,y,}$, m^*_z) and their corresponding values used for each valley are the same used in ref 10.

In Figure 2 is plotted the binding energy of a donor impurity in function of the length of the cylinder with an applied magnetic field of 20T and 50 T, with different values of the radii. It is observed that for a given radius, for example $1.4a_0^*$, the binding energy decreases when the cylinder height increases. Also it is observed that the binding energy of the impurity increases when the cylindrical radius is diminishing, for all values of the cylindrical height. For r_c = R, r_c is the cyclotron radius of a carrier in a magnetic field and R the radius of the cylinder, there is a limit for the transition from geometric confinement regime to the magnetic confinement regime of the carrier. When B = 20T, the cyclotron radius of an electron equals to a $r_c = \sqrt{\frac{1}{\gamma}} = 4.742\ a_0^*$, in that

way for the cylinder radii, $R<r_c$, the geometric confinement is greater than the magnetic confinement. The smaller radius of AlAs considered in this problem is $1.4a_0^*$, because for smallest values, the X_z valley is aligned with the first sublevel e_1 of the well GaAs and appears a mixture of bands, which is not considered in this paper.

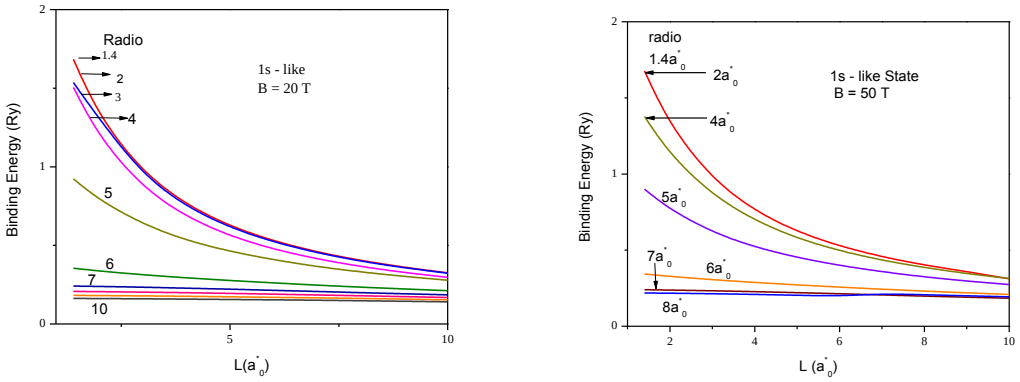

Figure 2. Graphic of the binding energy E_b of a donor impurity vs length of a quantum well for various radii and with an applied magnetic field of 20 T (left) and 50 T (right).

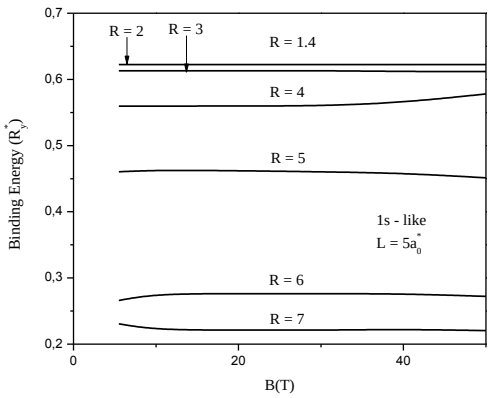

Figure 3. Ground state Binding energy for an impurity centered in the structure as a function of the applied magnetic field and different values for the wire radii, with cylindrical height $L=5a_0^*$.

Figure 3 shows the binding energy as a function of the magnetic field for a cylinder height of $5a_0^*$ and different values of the cylindrical radii. For a given magnetic field, the energy increases with decreasing radius of the cylinder and geometric confinement is more effective for smaller radii. With small cylinder radii the binding energy remains approximately constant.

4. Conclusion

Through the proposed model were calculated the energies E_z and E_ρ for the first level of a carrier in a quantum well in the z and directions and the total energy in the quantum well when applying different magnetic fields. We calculated binding energies of a donor impurity in a type II quantum dot in function of the well height for different radii of the cylinder and applied magnetic fields of 20T and 50T. The binding energy of the impurity, for a given radius of the cylinder decreases as the height of the cylinder increases. The binding energy of the impurity, for a given cylinder height increases as the radius of the cylinder decreases.

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