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Stark effect-dependent of ground-state donor binding energy in InGaN/GaN parabolic QWW

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ABSTRACT

Using the finite-difference method within the quasi-one-dimensional effective potential model and effective mass approximation, the ground-state binding energy of hydrogenic shallow-donor impurity in wurtzite (WZ) (In,Ga)N/GaN parabolic transversal-section quantum-well wires (PQWWs) subjected to external electric field is investigated. An effective radius of a cylindrical QWW describing the strength of the lateral confinement is introduced. The results show that (i) the position of the largest electron probability density in x–y plane is located at a point and it is pushed along the negative sense by the electric field directed along the positive sense, (ii) the ground-state binding energy is largest for the impurity located at this point and starts to decrease when the impurity is away from this point, (iii) the ground-state binding energy decreases with increase in the external electric field and effective radius, and (iv) the Stark-shift increases with the increase of the external electric field and the effective radius.

1. Introduction

With the development of experimental techniques and analytical methods, there has been a considerable amount of work devoted to study of the hydrogenic impurities-related electric properties in low-dimensional semiconductors heterostructures such quantum well (QW), quantum well wire (QWW) and quantum dot (QD) [1–16]. It is important to understand the electric and optical properties of impurities because the optical and transport properties of devices made from these materials are strongly affected by the existence of the hydrogenic impurities [2–7,17].

There are a number of studies concerning hydrogenic impurities in QWWs under external fields which are an interesting probe for studying the physical properties of low-dimensional systems both from theoretical and technological points of view. Dalgic and coworkers [18,19] have investigated the electric field effect on the non-hydrogenic binding energy of shallow donor impurity in a square and cylindrical GaAs/(Ga, Al)As QWW. In the same sense, Aktas and coworkers [13,14] have estimated the binding energy of shallow donor impurity under both electric and magnetic fields in a coaxial GaAs–Ga,AlAs QWW. These authors have calculated the binding energy as a function of the impurity position and barrier thickness for various values of electric and magnetic fields. An and Liu [20] have investigated the properties of hydrogenic impurities in a parabolic GaAs QWW in the presence of magnetic field. The analytical calculation of the eigenstates of QWWs is complicated or insoluble even due to the existence of the Coulombian potential and two-dimensional confinement. To overcome this problem, several numerical methods are suggested and adopted by different authors such the finite element method, the plane wave expansion, the variational method, the potential morphing method and the finite-difference method.

In this paper, based on the finite-difference method adopted in different works [21,22,23] and quasi-one-dimensional effective potential model, the calculation of the ground-state shallow donor binding energy in QWWs with lateral parabolic potential and electric field perpendicular to the z-axis growth direction is investigated.

2. Theoretical formalism

We consider that the hydrogenic shallow donor impurity is located at (x_i,y_i) in the (x,y)-plane which constitutes the lateral surface of parabolic quantum-well wire (PQWW) made out of WZ $In_vGa_{1-v}N$and surrounded by GaN barriers. In this situation, the electron is free to move in the z-axis longitudinal direction and is confined by parabolic lateral confinement along x-axis and y-axis. The effective-mass Hamiltonian of an electron in PQWW in the

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absence of the hydrogenic impurity for an electric field parallel to the x-axis can be expressed as follows:

$$H_0 = -\frac{\hbar^2}{2m^*}\Delta + \frac{1}{2}m^*\omega_0^2(x^2+y^2) + |e|Fx \quad (1)$$

e and m^* are the electron charge and the electron effective-mass respectively, ω_0 is the harmonic oscillator frequency and $F>0$ is the electric field.

In the linear approximation, the effective-mass in the PQWW is given as:

$$m^*_{InGaN} = v m^*_{InN} + (1-v)m^*_{GaN} \quad (2)$$

By adopting the effective Bohr radius (EBR) $a^* = \varepsilon^*\hbar^2/m^*e^2$ for the length unit, the effective electron Rydberg $R^* = e^2/2\varepsilon^* a^*$ as the unit of the energy and $F^* = e/\varepsilon^* a^{*2}$ as the unit of the electric field, the Hamiltonian (1) can be expressed as:

$$\widehat{H}_0 = -\Delta + \frac{r^2}{{r_e}^4} - {r_e}^4 F^2 \quad (3)$$

r_e is defined as the oscillator length which is given as:

$$r_e = \sqrt{\frac{\hbar}{m^*\omega_0}} \quad (4)$$

For a fixed finite parabolic potential ω_0, the value of the oscillator length can be modulated by the Indium fraction in the QWW.

In Eq. (3), r measures the electron distance from the origin of the wire along the z-axis under the electric field. It is given as:

$$r = \sqrt{\left(x + {r_e}^4 F\right)^2 + y^2} \quad (5)$$

We notice that the lateral confinement effect scales as $1/{r_e}^4$. It is also indicated that the confinement potential depends strongly on r_e, i.e., the smaller the r_e, the stronger the lateral confinement. Therefore, r_e is defined as an effective radius of the QWW cross section which is used to describe the lateral confinement in PQWW.

By solving the Schrodinger equation in cylindrical coordinates:

$$\widehat{H}_0\psi_0(r,\theta) = E_0\psi_0(r,\theta) \quad (6)$$

The exact solution has been obtained in this situation which leads us to the ground-state wave-function and energy. They are given respectively as:

$$\psi_0(r,\theta) = \frac{1}{\sqrt{\pi}r_e}\exp\left(-\frac{r^2}{2{r_e}^2}\right) \quad (7)$$

$$E_0 = \frac{2}{{r_e}^2} - {r_e}^4 F^2 \quad (8)$$

In the presence of the hydrogenic shallow-donor impurity, the Hamiltonian described in Eq. (3) becomes:

$$\widehat{H} = \widehat{H}_0 - \frac{2}{\varepsilon^* r_i} \quad (9)$$

ε^* is the mean dielectric constant and r_i is the electron–impurity distance in which x_i and y_i are the coordinates of the impurity in the PQWW. They are given as:

$$r_i = \sqrt{(x-x_i)^2 + (y-y_i)^2 + z^2} \quad (10)$$

$$\varepsilon^*(In_vGa_{1-v}N) = v.\varepsilon^{InN} + (1-v)\varepsilon^{GaN} \quad (11)$$

In this problem, there is no exact solution for the combination of parabolic confinement potential and Coulombian interaction. However, in the present situation we have adopted the same method used in Ref. [24] in which the authors have proposed an analytical 1D formula for the effective interaction potential between confined carriers. For a bound electron-hole pair exciton in a parabolic quantum wire, the obtained ground state energy using the analytical 1D formula is very close to the exact one. So, the calculation of the eigenstates in 1D model is solved exactly with the effective interaction potential in this case. Then, it is permissible to replace the Colombian potential with the effective potential energy $V_{eff}(z)$ [24]. Within this approximation, in the cylindrical coordinates the Hamiltonian can be separated as follows:

$$H = H_\perp + H_{//} \quad (12)$$

$H_\perp$ is the perpendicular Hamiltonian which is the same as one given in Eq. (1) ($H_\perp = H_0$) and $H_{//}$ is the parallel Hamiltonian given as:

$$H_{//} = -\frac{\partial^2}{\partial z^2} - V_{eff}(z) \quad (13)$$

The effective potential energy $V_{eff}(z)$ is defined as:

$$V_{eff}(z) = \int_{-\infty}^{+\infty} |\psi_0(x,y)|^2 . \frac{2}{\varepsilon^* r_i} dxdy \quad (14)$$

This integral is calculated as in Ref. [24] by replacing the lateral probability density ($|\psi_0(x,y)|^2$) and the Coulombian potential by their Fourier transforms and integrating over the transverse coordinates and transverse momenta. Then, the effective potential energy becomes:

$$V_{eff}(z) = 2\int_0^{+\infty} J_0\left(u\sqrt{\left({r_e}^4F^2 - x_i\right)^2 + {y_i}^2}\right)\exp\left(-\frac{{r_e}^2}{4}u^2 - u|z|\right)du \quad (15)$$

J_0 is the zeroth order Bessel function and $|\psi_0(x,y)|^2$is the electron ground-state probability density without the presence of the impurity in the QWWs. Using Eq. (7), one can obtain:

$$|\psi_0(x,y)|^2 = \frac{1}{\pi {r_e}^2}\exp\left(-\frac{\left(x + {r_e}^4F\right)^2 + y^2}{{r_e}^2}\right) \quad (16)$$

The eigenvalues of the Hamiltonian given in Eq. (13) can be obtained using the finite-difference method on a one-dimensional mesh. The ground state energy with the presence of the impurity is:

$$E_I = E_0 + E_{//} \quad (17)$$

And then, the ground state binding energy is obtained as follows:

$$E_b = E_0 - E_I = -E_{//} \quad (18)$$

3. Results and discussion:

It is well known that the electron–impurity distance is the main parameter which affects the binding energy strongly. To clarify the binding energy dependency, it is necessary to study the electron probability density without the presence of the impurity. For $In_{0.2}Ga_{0.8}N$, the effective units used in this paper are $a^* = 2.80$ nm, $R^* = 26.65$ meVand $F^* = 0.18$ MV/cm.

In Fig. 1(a), we present the ground-state probability density of electron in (x,y)-plane without the impurity in the QWW. One can see that $|\psi_0(x,y)|^2$ diminishes slightly and moves along the x-axis as a function of the electric field directed along the x-axis. It is clear that its amplitude is less affected than its displacement along the electric field axis. The larger the electric field is, the more the displacement is marked and its maximum is obtained at a point. To clarify the effective radius effect, we have plotted in Fig. 1(b) the combined effect of effective radius and electric field. We have only taken account of this later to separate the probability densities curvatures along the x-axis. It is shown that