Electric field Effect on Lowest Excited-State Binding Energy of Hydrogenic Impurity in (In,Ga)N Parabolic Wire

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Externally applied electric field and effective radius effects are investigated on the lowest excited-state shallow-donor binding energy in (In,Ga)N-GaN parabolic wire within the framework of single band effective-mass approximation. The calculations are performed using the finite-difference method within the quasi-one-dimensional effective potential model. Our results reveal that: (i) the probability density is the largest on a circularity whose radius is the effective radius, (ii) the lowest excited-state binding energy is the largest for impurity located on this circularity while it starts to decrease when the impurity is away from the circularity and (iii) the binding energy is strongly-dependent on the complex interplay of spatial confinement, coulomb interaction and applied electric field.

1. Introduction

In the recent years, a great attention has been devoted to the study and engineering of high quality devices of very low-dimensional systems (LDS) such as quantum well (QW), quantum well wire (QWW), quantum dot (QD) and quantum ring (QR). External perturbation such electric field, magnetic field, hydrostatic pressure and temperature on the physics of LDS constitutes a subject of considerable interest from both theoretical and experimentally, due to their importance in the development of new semiconductor devices and applications. Therefore, the study of the impurity states in semiconductor is imperative as the incorporation of impurities can dramatically change the performance of optoelectronic devices. The application of an externally electric field in particularly along the growth direction of the heterostructure gives rise to a polarization of the carrier distribution with a consequent energy shift of the quantum states. Such effects may induce considerable changes in the energy spectrum of the carriers which could be used to control and modulate the output of optoelectronic devices. There are many works related to theoretical investigation of the electric field effects on the electronic states and optical properties [1–12].

Using variational approach, the investigation of electric field effect on non-hydrogenic binding energy in cylindrical and square GaAs wire is reported in Refs. [13,14]. It is found that the binding energy diminishes as a function of electric field strength in particularly for large wire. For cylinder InGaN-GaN wire and based on the plane-wave basis in the framework of effective-mass envelope-function theory, the ground-state binding energy is calculated under electric field effect [15]. It is reported that the shallow-donor binding energy is highly dependent external electric field. It is also shown that the applied electric field enhances the Stark-shift. Recently, for the same wire-shape, we have examined this effect on the ground-state shallow donor binding energy [4] using the finite-difference method.We have obtained that the binding energy (Stark−Shift) decreases (increases) as a function of electric field. Our attention is to expand this study to the excited-states in (In,Ga)N-GaN LDS.

In the present paper, based on the finite-difference method within the quasi-one dimensional effective potential model and within the approximation of single band effectivemass, externally applied electric field and effective radius effects are investigated on the binding energy of lowest-excited state (2S) of confined donor in (In,Ga)N parabolic quantum well wire (PQWW).

2. Theoretical formalism

Let us to consider hydrogenic shallow-donor impurity located at (x_i, y_i) in the lateral area of WZ $In_\nu Ga_{1-\nu}N$-GaN PQWW. Within the effective-mass approximation and without impurity, the Hamiltonian of an electron under uniform electric field perpendicular to z-axis can be given by the following expression

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

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.

Based on the effective units, effective Bohr radius (EBR) $a^* = \varepsilon_0\hbar^2/m^*e^2$ for the length, effective electron Rydberg $R^* = e^2/2\varepsilon_0 a^*$ for the energy and effective field electric $F^* = e/\varepsilon^* a^{*2}$ for electric field, the effective Hamiltonian becomes

$$\widehat{H}_0 = -\nabla^2 + \frac{r^2}{r_e^4}. \quad (2)$$

In Eq. (2), r_e is the oscillator length while r is the distance between electron and the z-axis in the presence

of externally electric field:

$$r_e = \sqrt{\frac{\hbar}{m^* \omega_0}}, \tag{3}$$

$$r = \sqrt{\left(x + r_e^4 F^2 \cos^2(\theta)\right)^2 + \left(y + r_e^y F^2 \sin^2(\theta)\right)^2}. \tag{4}$$

It is clear that for a given finite parabolic potential ω_0, r_e can be controlled by the In-fraction inside the wire. It is interesting to note that the lateral confinement effect scales as $1/r_e^4$. The greater the r_e is, the weaker is the lateral confinement. Thus, r_e is considered as the effective radius (ER) of the wire cross section which describes the lateral confinement.

The lowest-excited energy and the corresponding wave-function are obtained by the exact solution of the Schrödinger equation ($\widehat{H}_0 \psi_0^{\text{ex}} = E_0^{\text{ex}} \psi_0^{\text{ex}}$). They are obtained respectively as:

$$\psi_0^{\text{ex}}(r, \theta) = \frac{r}{\sqrt{\pi} r_e^e} \exp\left(-\frac{r^2}{2 r_e^2}\right) \exp(i\theta), \tag{5}$$

$$E_0^{\text{ex}} = \frac{4}{r_e^2} - r_e^4 F^2. \tag{6}$$

In the presence of impurity, the exact solution of the problem is impossible. Then, we have used the same method as that adopted for the ground-state in Refs. [4,16] and for the lowest excited-state [17] in which an analytical 1D formula for the effective interaction potential between confined carriers is proposed. Then, we can replace the Coulomb interaction potential with the effective potential energy $V_{\text{eff}}^{\text{ex}}(z)$. Within this formalism, the Hamiltonian can be separated in cylindrical coordinates and can be given as

$$\bar{H}_F^{Imp} = \widehat{H}_{x,y} + \widehat{H}_z, \tag{7}$$

$\widehat{H}_{x,y}$, y is equal to effective Hamiltonian ($\widehat{H}_0$) while $\widehat{H}_z$ is given as

$$\widehat{H}_z = -\frac{\partial^2}{\partial z^2} - V_{\text{eff}}^{\text{ex}}(z). \tag{8}$$

The effective potential energy $V_{\text{eff}}^{\text{ex}}(z)$ is given as:

$$V_{\text{eff}}^{\text{ex}}(z) = 2 \int_0^{+\infty} \left(1 - \frac{u^2 r_e^2}{4}\right) \times J_0\left(u \sqrt{\left(r_e^4 F^2 \sin^2(\theta) - y_i\right)^2 + \left(r_e^4 F^2 \cos^2(\theta) - x_i\right)^2}\right) \times \exp\left(-\frac{r_e^2}{4} u^2 - u|z|\right) du. \tag{9}$$

J_0 is the zeroth-order Bessel function.

Then, the lowest-excited state shallow-donor binding energy is obtained as follows

$$E_b = E_0^{\text{ex}} - E_F^{Imp} = -E_z. \tag{10}$$

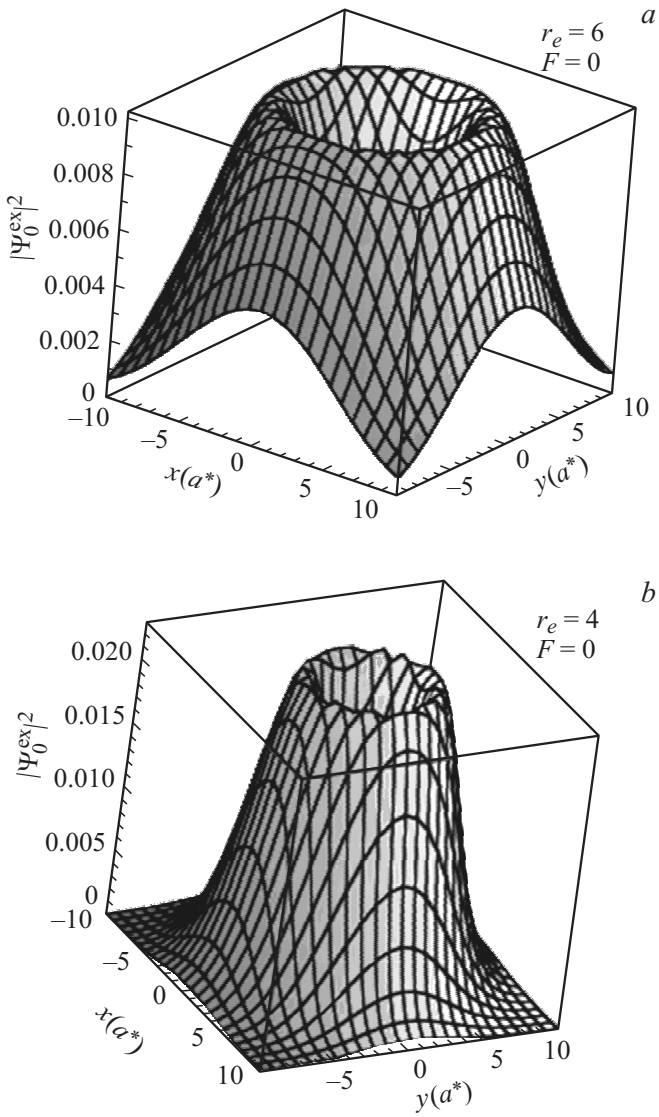

Figure 1. *a, b* — the lowest-excited state probability density in lateral cross section without electric field effect for two effective radii.

3. Results and discussion

It is well known that electron-impurity correlation is the main factor which affects the binding energy. To get a good picture of its dependency, the electron lateral probability density (LPD) without the presence of the impurity is presented under externally electric field and effective radius effects. For $In_{0.2}Ga_{0.8}N$, the effective units used in this paper are $a^* = 2.80$ nm, $R^* = 26.65$ meV and $F^* = 18\,\text{MV} \cdot \text{m}^{-1}$.

In Fig. 1, *a, b* we present the lowest-excited state LPD in (x, y)-plane without the impurity in the PQWW and without externally applied electric field. It is shown that the LPD is the smallest at the axis center of wire. The LPD increases as the distance from the center increases. For the distance equal to r_e, the LPD is maximum and then decreases as

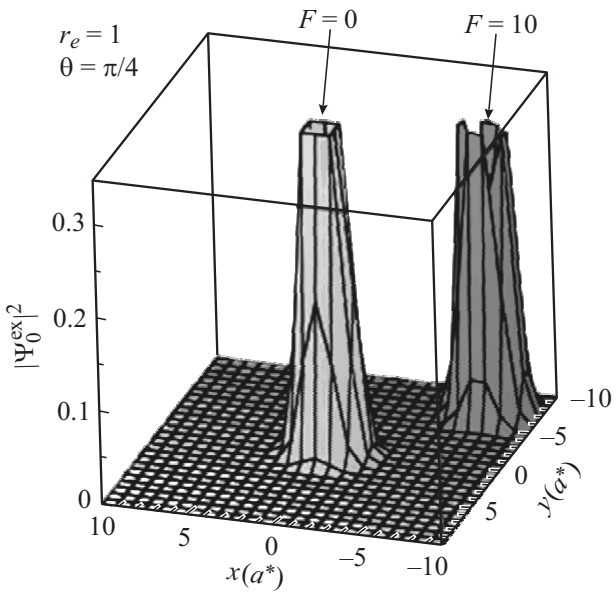

Figure 2. The lowest-excited state probability density in lateral cross section for two values of the applied electric field.

the distance increases. It appears also that the maximum of the LPD diminishes as the effective radius increases. The dependency of LPD versus externally electric field is shown in Fig. 2. It is found that for $\theta = \pi/4$, the maximum of LPD moves along the diagonal-axis of the lateral area, i. e., the LPD moves in the opposite sense of the applied electric field. It is also shown that the maximum of LPD decreases when the electric field increases.

Fig. 3 depicts the combined effect of electric field and effective radius on the lowest-excited state shallow-donor binding energy versus the impurity position along x-axis. The same results are obtained for the impurity situated along y-axis (not shown here). When the electric field is not applied, we can see that as the effective radius increases, the binding energy decreases especially for the impurity located close to the center-axis. For the impurity located away from the center axis, the effective radius effect is less sensitive. It appears also that the binding energy is the largest for the impurity located at $x_i = \pm r_e$. This result is in good agreement with that presented on Fig. 2, i. e., the distance between electron and the impurity located at $x_i = \pm r_e$ is the shortest and then the binding energy is the largest. For $|x_i| < r_e$, the binding energy increases as a function of $|x_i|$ to reach its maximum at $|x_i| = r_e$ and then decreases for $|x_i| > r_e$. When the electric field is applied along the positive (negative) x-axis direction, the typical symmetric behavior is broken and the binding energy diminishes for all effective radii. It is also shown that the maxima of the binding energy moves to negative (positive) x-axis direction. This result can be explained by the displacement of the LPD along the opposite sense of the electric field direction. We note also that such displacement is governed by the strength of electric field, its direction and the effective radius. For a given electric field, the more the r_e increases the more the displacement to the opposite sense is marked. According to Fig. 3, two confinement regimes are obtained. For moderate confinement regime ($r_e \geq 1$), the binding energy presents two maxima situated at $x_i = \pm r_e$ while for strong confinement regime ($r_e < 1$) one peak is depicted. It appears also that the electric field effect is not the same for all effective radii but depends strongly on the confinement regime, i. e., the maxima displacement and the decreasing of the binding energy become less sensitive to electric field effect for strong confinement.

It is interesting to mention that the results reported in the literature corresponding to electric field effect on different LDS-shapes are in good agreement with those presented above. For example, it is obtained in Refs. [18,19] that the ground-state binding energy decreases under external electric field effect in GaAs SQD surrounded by (Ga,Al)As matrix for different confinement especially for the moderate confinement regime (Fig. 2 [18]) while this effect is less sensitive for strong confinement (Fig. 2 [19]). Incidentally, Pan et al. [20] have reported the impurity states in GaAs-(Al, Ga)As cylindrical QD in the presence of electric field. As a general feature, they have shown that the interplay of the spatial confinement and electric field confinement on the electron and the shallow-donor in the QD leads to complex behavior of the binding energy, i. e., the electric field effect depends strongly of the positions of the impurity and the CQD dimension.

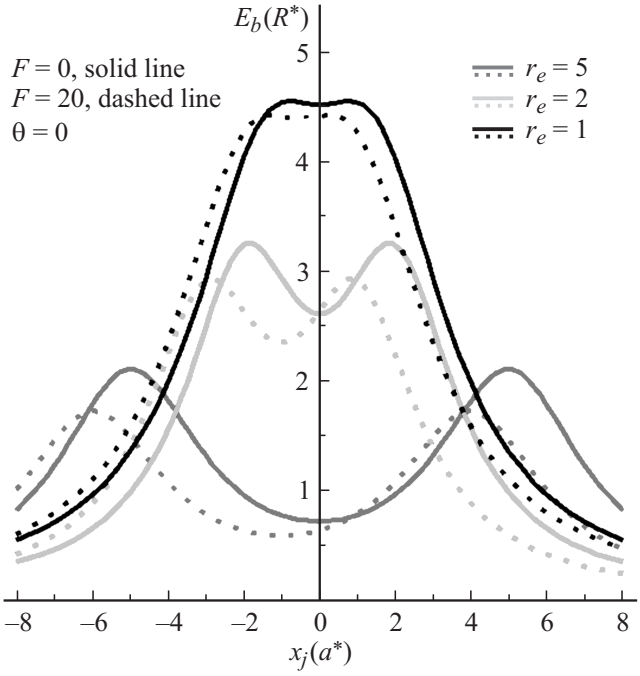

Figure 3. The lowest-excited state shallow-donor binding energy as a function of the impurity's position located along x-axis in $In_{0.2}Ga_{0.8}N$ PQWW. The combined effect of effective radius and electric field is reported.

4. Conclusion

Using the finite-difference method within the quasi-one-dimensional effective potential model and within the effective-mass approximation, we have investigated the effective radius, impurity's position and electric field effects on the lowest-excited state binding energy. Important changes of the binding energy have observed. It is obtained that:

— The binding energy is the largest for impurity located on the circularity corresponding to the maximum of LPD.

— The binding energy drops as the impurity is away from this circularity.

— The binding energy is dependent on the complex interplay of spatial confinement, Coulomb interaction (position of the impurity) and applied electric field effect.

References

[1] S. Baskoutas, A.F. Terzis. Eur. Phys. J. B, **69**, 237 (2009).
[2] S. Baskoutas, A.F. Terzis, J. Comput. and Theor. Nanosci., **7**, 492 (2010).
[3] Z. Zeng, C.S. Garoufalis, S. Baskoutas. J. Phys. D: Appl. Phys., **45**, 235 102 (2012).
[4] H. El Ghazi, I. Zorkani, A. Jorio. Physica B: Condens. Matter, **412**, 87 (2013).
[5] E. Sadeghi. Physica E, **41**, 1319 (2009).
[6] P. Baser, S. Elagoz, D. Kartal, H.D. Karki. Superlat. Microstr., **49**, 497 (2011).
[7] H. El Ghazi, A. Jorio, I. Zorkani. Physica B: Condens. Matter, **410**, 49 (2013).
[8] P. Baser, S. Elagoz, N. Baraz. Physica E, **44**, 356 (2011).
[9] C. Xia, Z. Zeng, S. Wei. J. Appl. Phys., **107**, 014 305 (2010).
[10] N. Esuanu, E.C. Niculescu, L.M. Bureleanu. Physica E, **41**, 1386 (2009).
[11] E.C. Niculescu, A. Lupascu, L.M. Burileanu. U.P.B. Sci. Bull., **71**, 45 (2009).
[12] P. Baser, I. Altuntas, S. Elagoz. Fen Bilimleri Derg., **23**, 171 (2011).
[13] S. Dalgic, M. Ulas, B. Ozkapi. J. Optoelectron. Adv. Mater., **7**, 2041 (2005).
[14] S. Dalgic, B. Ozkapi. J. Optoelectron. Adv. Mater., **11**, 2120 (2009).
[15] H. Wang, L. Jiang, Q. Gong, S. Feng. Physica B, **405**, 3818 (2010).
[16] S. Bednarek, B. Szafran, T. Chwiej, J. Adamowski. Phys. Rev. B, **68**, 045 328 (2003).
[17] H. El Ghazi, A. Jorio, I. Zorkani. Commun. Phys., **23**, 275 (2013).
[18] S.J. Gerardin, K. Navaneethakrishnan. Sol. St. Commun., **126**, 681 (2003).
[19] A.J. Peter, K. Navaneethkrishnan. Superlat. Microstr., **43**, 63 (2008).
[20] P. Jiang-Hong, L. Li-Zhe, L. Min. Chin. Phys. Lett., **28**, 086 201 (2011).

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