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Exciton binding energy in a pyramidal quantum dot

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Abstract. The effects of spatially dependent effective mass, non-parabolicity of the conduction band and dielectric screening function on exciton binding energy in a pyramid-shaped quantum dot of GaAs have been investigated by variational method as a function of base width of the pyramid. We have assumed that the pyramid has a square base with area $a \times a$ and height of the pyramid $H = a/2$. The trial wave function of the exciton has been chosen according to the even mirror boundary condition, i.e. the wave function of the exciton at the boundary could be non-zero. The results show that (i) the non-parabolicity of the conduction band affects the light hole (lh) and heavy hole (hh) excitons to be more bound than that with parabolicity of the conduction band, (ii) the dielectric screening function (DSF) affects the lh and hh excitons to be more bound than that without the DSF and (iii) the spatially dependent effective mass (SDEM) affects the lh and hh excitons to be less bound than that without the SDEM. The combined effects of DSF and SDEM on exciton binding energy have also been calculated. The results are compared with those available in the literature.

Keywords. Pyramid quantum dot; dielectric screening function; spatially dependent effective mass; exciton; GaAs; non-parabolicity.

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1. Introduction

Due to the vast development in the field of nanotechnology, the problems of low-dimensional semiconducting systems achieved immense interest in the past few years. The advanced techniques of nanotechnology have made carrier confinement to be possible in a quantum dot (QD) with different shapes. These structures may generate unique properties and they show immense potential in the field of opto-electronic device fabrication [1].

Theoretical investigations on hydrogenic donor and exciton in quantum nanostructures made of semiconductors play an important role in understanding the electrical and optical properties of the nanostructures [2,3]. Theoretical and experimental studies on exciton binding energy have been reported for cylindrical QD [4], spherical QD [5], rectangular and parabolic QDs [6]. The results confirmed that strong confinement leads to more bounded excitons.

Spatially dependent effective mass (SDEM) and dielectric screening function (DSF) affect the exciton binding energy. Effect of the dielectric function on exciton binding energy in GaAs and $GaAs/Ga_{1-x}Al_xAs$ superlattices has been studied as a function of well width [7]. The effect of DSF on binding energies of the donor, acceptor and exciton in finite quantum well (QW) of GaAs/GaAlAs has been demonstrated in the presence of magnetic field [8]. Deng *et al* [9] have calculated the effect of spatial variation of dielectric screening on binding energy of impurity states in a spherical QD as a function of dot radius. Effect of SDEM on hydrogenic impurity binding energy in a finite parabolic QW has been studied as a function of well width by Qi *et al* [10]. Peter and Navaneethakrishnan [11] have investigated the effects of both SDEM and DSF on hydrogenic donor binding energy in a QD of GaAs/GaAlAs.

Another important effect which should be taken into account is non-parabolicity of the conduction band without which the result will have a significant error. Nomura and Kobayashi [12] have compared the Coulomb energy as a function of size of the CdSe microcrystallite with and without the effect of non-parabolicity of conduction band. The effects of conduction band non-parabolicity

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on effective masses of electron and exciton in QD and ultrathin QW made of GaAs/AlGaAs have been found experimentally and compared with theoretical model by Schildermans *et al* [13]. Sidor *et al* [14] have investigated exciton diamagnetic shift in QW and quantum wire InAs/InP theoretically and experimentally as a function of magnetic field and proved that the results from the theoretical values using non-parabolicity effective mass of electron, fitted well with the results obtained experimentally. Andreani and Pasquarello [15] have determined theoretically the effects of non-parabolicity of the conduction band and dielectric constant mismatch of the well and the barrier materials on exciton binding energy in $GaAs/Ga_{1-x}Al_xAs$ QWs as a function of well width. Exciton binding energy in a QW of $GaAs/Ga_{1-x}Al_xAs$ have been calculated using perturbational approach by including valence band coupling and non-parabolicity by Ekenberg and Altarelli [16].

The evolution of growth techniques of low-dimensional nanostructures allows the production of QD with pyramid-like shape. Studies on pyramidal QD have been emerging in the literature. Energy spectrum of electron states in a pyramid QD of GaAs has been calculated as a function of vertex angle by Lozovski and Piatnytsia [17]. Vorobiev *et al* [18] have studied the energy spectra of an electron in a pyramidal QD with even mirror boundary condition. Effect of aspect ratio of the pyramid QD (ratio of height of the pyramid to the side of the base) on the energy of optical transitions has been determined by Vorobiev *et al* [19]. Grundmann *et al* [20] have investigated the strain distribution, optical phonons and electronic structure in InAs/GaAs pyramidal QD. The effect of temperature on the strain and band structure of $In_xGa_{1-x}As$ QD with pyramidal shape has been studied by Borji *et al* [21].

In the present paper, we made an attempt to study the effects of DSF, SDEM and conduction band non-parabolicity on exciton binding energy in a pyramid QD shaped as a square base with even boundary condition. We have used variational method to calculate the binding energy.

2. Theory and formulation

The Hamiltonian for an exciton in a pyramidal QD can be written in effective Rydberg as

$$\mathcal{H} = -\frac{\mu_{ih}^*}{m_e^*}\frac{\partial^2}{\partial x_e^2} - \frac{\mu_{ih}^*}{m_{ih}^*}\frac{\partial^2}{\partial x_h^2} - \frac{\mu_{ih}^*}{m_e^*}\frac{\partial^2}{\partial y_e^2} - \frac{\mu_{ih}^*}{m_{ih}^*}\frac{\partial^2}{\partial y_h^2} - \frac{\mu_{ih}^*}{m_e^*}\frac{\partial^2}{\partial z_e^2} - \frac{\mu_{ih}^*}{m_{ih}^*}\frac{\partial^2}{\partial z_h^2} - \frac{2}{r} + V(x, y, z), \quad (1)$$

where

$$r = \sqrt{(x_e - x_h)^2 + (y_e - y_h)^2 + (z_e - z_h)^2}.$$

μ_{ih}^* is the reduced effective mass of the exciton given by

$$\frac{1}{\mu_{ih}^*} = \frac{1}{m_e^*} + \frac{1}{m_{ih}^*}. \quad (2)$$

The effective Bohr radius ($a^* = \hbar^2\varepsilon_0/\mu_{ih}^* e^2$) and the effective Rydberg ($R^* = \mu_{ih}^* e^4/2\hbar^2\varepsilon_0^2$) are used as the units of length and energy respectively.

2.1 *Non-parabolicity of the conduction band*

The non-parabolicity of the conduction band can be defined by the energy-dependent effective mass [22]

$$m_e^*(E_e) = 0.0665 \times \left(1 + \frac{0.0436E_e + 0.236E_e^2 - 0.147E_e^3}{0.0665}\right),$$

where E_e is the ground-state energy of the electron in eV.

2.2 *Dielectric screening function*

The dielectric screening function (DSF) [11] can be expressed as

$$\frac{1}{\varepsilon(r)} = \frac{1}{\varepsilon_0} + \left(1 - \frac{1}{\varepsilon_0}\right)\exp\left(-\frac{r}{c}\right), \quad (3)$$

where ε_0 is the static dielectric constant of GaAs and c is the screening constant which is taken to be 0.058 nm. When the DSF is included, the interaction term in the Hamiltonian $2/r$ changes as

$$\frac{2}{r}\left[1 + (\varepsilon_0 - 1)\exp\left(-\frac{r}{c}\right)\right].$$

2.3 *Spatially dependent effective mass*

For a barrier model, SDEM [11] is given by

$$\frac{1}{m(r)} = \frac{1}{m^*} + \left(1 - \frac{1}{m^*}\right)\exp(-\zeta r), \quad (4)$$

where m^* is the effective mass of the carrier and ζ is a constant which is taken to be 0.01 a.u. This value is chosen because as $r \to 0$, the particle is strongly bound within the δ function well and as $r \to \infty$, the system becomes 3D.

2.4 *Pyramidal quantum dot*

Figure 1 shows the shape of the pyramidal QD with square base $a \times a$. Here, a is the side of the square

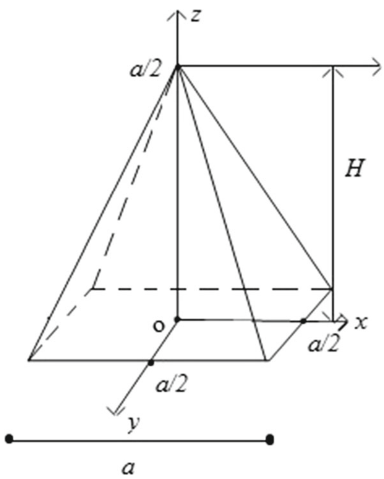

Figure 1. The geometry of the pyramidal quantum dot.

base and H is the height of the pyramid which is taken to be $a/2$. The mirror reflection boundary conditions have been proposed in order to find the solution of the Schrödinger equation for triangular and hexangular dots [18] and they are even and odd mirror boundary conditions. In the case of odd mirror boundary conditions, the wave function at the boundary could be zero, i.e. the particle cannot penetrate into the barrier and this situation corresponds to the case of strong confinement. The even mirror boundary condition describes the weak confinement, when a particle can penetrate into the barrier and return into the confined volume, i.e. the wave function at the boundary could be non-zero. In this work, we consider even mirror boundary conditions.

The trial wave function for the ground-state exciton in a pyramidal QD with even mirror boundary condition is taken to be of the form [18]

$$\begin{aligned}\Psi = N\Big[&\cos\left(k\left(x_e-\frac{a}{2}\right)\right)\\ &+\cos\left(k\left(y_e-\frac{a}{2}\right)\right)+\cos(kz_e)\Big]\\ &\times\Big[\cos\left(k\left(x_h-\frac{a}{2}\right)\right)+\cos\left(k\left(y_h-\frac{a}{2}\right)\right)\\ &+\cos(kz_h)\Big]\mathrm{e}^{-\lambda r},\end{aligned} \tag{5}$$

where λ is the variational parameter and N is the normalisation constant. $\langle\mathcal{H}\rangle$ is evaluated as a function of the variational parameter using the Hamiltonian in eq. (1) and the trial wave function in eq. (4) as

$$\langle\mathcal{H}\rangle = \frac{\int \Psi^*\mathcal{H}\Psi\ \mathrm{d}\tau}{\int \Psi^*\ \Psi\mathrm{d}\tau}. \tag{6}$$

The binding energy (E_B) of the exciton is then given by

$$E_B = E_e + E_h - \langle\mathcal{H}\rangle_{\min}, \tag{7}$$

where $\langle\mathcal{H}\rangle_{\min}$ is the minimised value of $\langle\mathcal{H}\rangle$ with respect to the variational parameter λ. E_e and E_h are the ground-state energies of the electron and the hole respectively in bare pyramidal QD calculated from

$$E_i = \frac{\hbar^2k^2}{2m_i} \quad \text{and} \quad k = \frac{2\pi}{a}.$$

3. Results and discussion

The parameters for GaAs [23] used in the calculations are (i) effective masses of hh, $m^*_{hh} = 0.34\,m_0$, lh, $m^*_{lh} = 0.094\,m_0$ and electron, $m^*_e = 0.0665\,m_0$; (ii) reduced masses of lh-exciton, $\mu^*_{lh} = 0.05562\,m_0$ and hh-exciton, $\mu^*_{hh} = 0.03895\,m_0$, where m_0 is the free electron mass; (iii) dielectric constant $\varepsilon_0 = 13.2$.

In figure 2, we have displayed the variation of lh and hh exciton binding energies in a pyramidal QD as a function of length of pyramid base a while the height of the QD is $a/2$. It is observed that the binding energy increases as length of the base decreases for both hh and lh. This is due to the compression of exciton wave function in the pyramidal QD.

It is also noted that the lh-exciton binding energy is lesser than that of hh-exciton for a given value of a. The difference in binding energy for lh and hh excitons is more pronounced only for $a < 4$ nm. A comparison of binding energies of excitons in GaAs pyramidal QD with the results of that in InAs pyramidal QD reported by Grundmann *et al* [20], shows that the binding energy in GaAs pyramidal QD is slightly larger than that in InAs for a given pyramid base length. Results for $a < 4$ nm and exclusive results for lh and hh excitons are not available in their paper for better comparison.

The effect of the conduction band non-parabolicity on binding energy of lh and hh exciton is presented in figures 3 and 4 respectively. It is observed that the

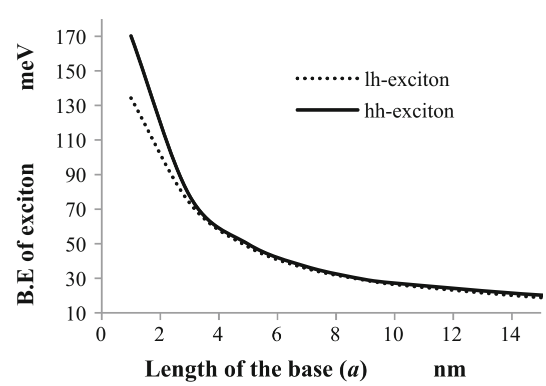

Figure 2. Exciton binding energy as a function of length of the base.

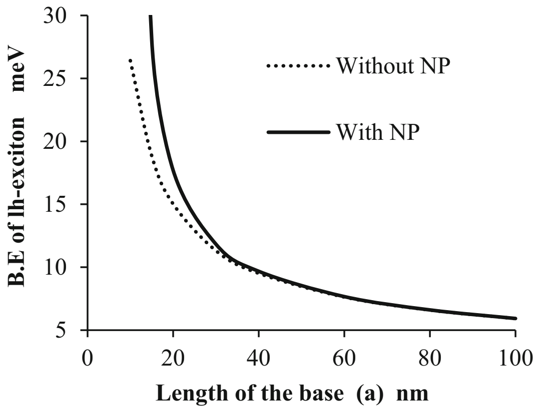

Figure 3. Binding energy of lh-exciton with and without the effect of non-parabolicity of the conduction band.

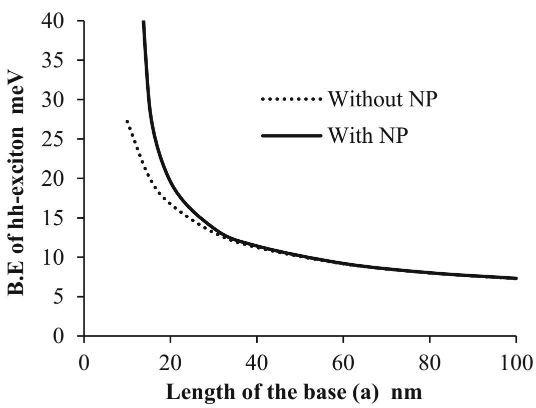

Figure 4. Binding energy of hh-exciton with and without the effect of non-parabolicity of the conduction band.

binding energy of the exciton increases when the non-parabolicity of the conduction band is included. This may be due to the enhancement of effective mass of the electron during the inclusion of non-parabolicity of the conduction band. For both lh and hh excitons, it is important to note that the effect of non-parabolicity is negligible for large base length (above 40 nm) of the pyramidal QD and it is important for small base length (below 40 nm). This behaviour is qualitatively similar to the case of quantum well of GaAs [15,16]. But the values of binding energy in this QD are larger than those in QW, which implies that the conduction band non-parabolicity affects a QD more than a QW, due to the confinement of exciton in 3D.

Figure 5 shows the variation of lh exciton binding energy as a function of a, for four different cases: (i) without DSF and SDEM, (ii) with DSF, (iii) with SDEM and (iv) with DSF and SDEM. It is seen from the figure that the inclusion of DSF increases the lh-exciton binding energy only for small a upto 4 nm, and above that the binding energy is insensitive to DSF and this

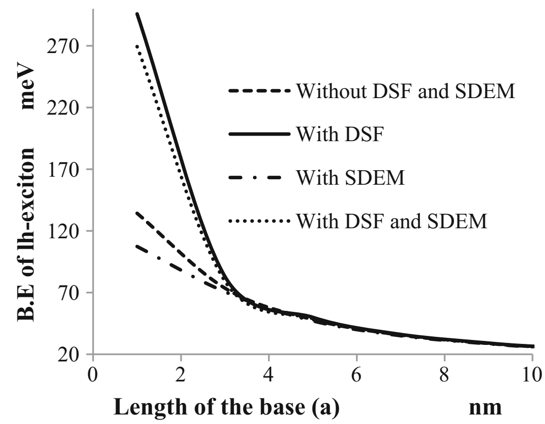

Figure 5. Binding energy of lh-exciton with the effects of DSF and SDEM.

behaviour is the same as in the case of exciton in finite GaAs/GaAlAs QW [8] and impurity states in spherical QD [9].

Another important result is that the inclusion of SDEM decreases the lh-exciton binding energy for small a. There is no appreciable change in binding energy when the effective mass varies with spatial distance between the electron and the hole for large pyramid base length. Hence the SDEM is insignificant for large sized pyramid. The effect of SDEM on the binding energy of the exciton is in contrast with that of the donor, in a parabolic QW [10] and quantum dot [11], because the average reduced mass of the exciton decreases due to the effect of SDEM but in the case of the donor, the effective mass increases. Studies on the effect of SDEM on exciton binding energy is sparse in the literature to compare our results. The combined effects of SDEM and DSF cause the binding energy to be larger than that of excluding the DSF and SDEM and are lesser than that of including the DSF only.

The effects of DSF and SDEM on hh-exciton binding energy are shown in figure 6. It is observed that there is no appreciable change in binding energy when the SDEM is included for hh-exciton. But, as in the case of lh-exciton, binding energy of hh-exciton increases by varying the dielectric constant with respect to the radius.

The effect of conduction band non-parabolicity on exciton binding energy is not studied along with the effects of DSF and SDEM because of the difference in the range of a in which these effects are pronounced.

Figures 7 and 8 respectively show the variation of differences in binding energy of lh and hh-exciton between the cases including and excluding DSF and SDEM. It is noted that, for both the cases of lh-exciton and hh-exciton, for the inclusion of DSF and inclusion of both DSF and SDEM, the binding energy changes markedly

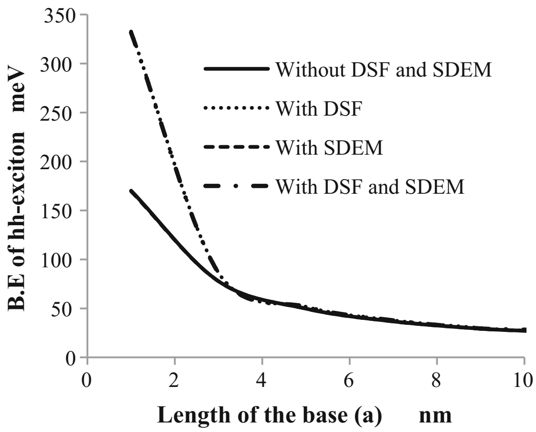

Figure 6. Binding energy of hh-exciton with the effects of DSF and SDEM.

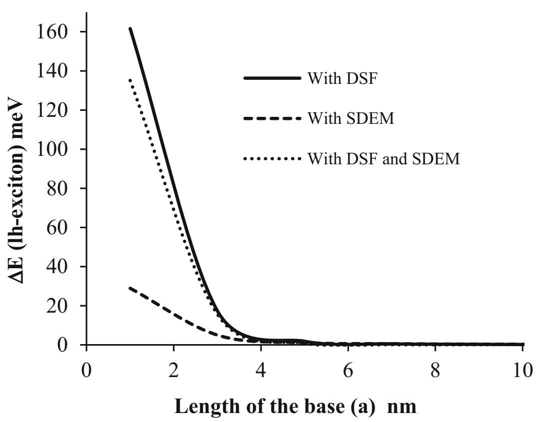

Figure 7. Difference in binding energy of lh-exciton including and excluding the effects of DSF and SDEM.

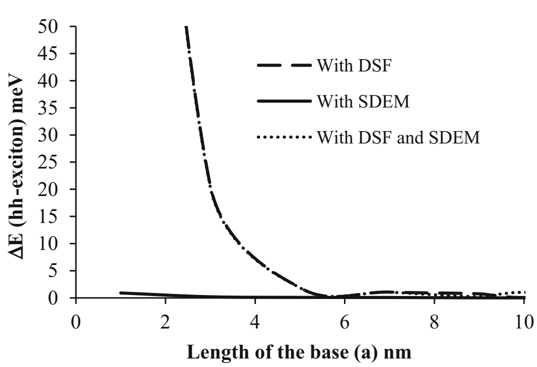

Figure 8. Difference in binding energy of hh-exciton including and excluding the effects of DSF and SDEM.

upto 4 nm and beyond that the changes in binding energy is nearly zero. It is also noted that, for the inclusion of SDEM, variation of binding energy of lh-exciton is larger than that of hh-exciton. In the case of hh-exciton, the difference in binding energy between the cases including and excluding SDEM is very small, about 0.6 meV.

4. Conclusion

We have investigated the lh and hh-exciton binding energy in a pyramidal QD of GaAs with even mirror boundary conditions with and without non-parabolicity of the conduction band. The results imply that the exciton binding energy with non-parabolicity is larger than that with parabolicity. Hence, crafting the conduction band of the quantum dot material as non-parabolic leads to enhanced binding energy. The individual and combined effects of DSF and SDEM on exciton binding energy in pyramidal quantum dot are also studied and the results are as follows: (i) when the DSF is included, the binding energy of the exciton increases, (ii) when the SDEM is included, the binding energy of exciton decreases, (iii) when DSF and SDEM are included, the binding energy becomes smaller than that with DSF and larger than that with SDEM. The variation of binding energy of the exciton with respect to DSF and SDEM occurs only for strong confinement and it remains unchanged for large confinement, i.e. above 4 nm. Hence, the SDEM for exciton binding energies in a pyramidal quantum dot with suitable DSF will be more fascinating in the probe of interband quantum dot laser that employ optical transitions between valence and conduction bands.

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