REVISTA COLOMBIANA DE FÍSICA, VOL. 37, No. 1. 2005

ELECTRON-HOLE PAIR IN A QUANTUM PYRAMID

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ABSTRACT

Variational calculation of the ground state energies of an exciton in $In_yAl_{1-y}As/Al_xGa_{1-x}As$ quantum pyramid is presented. To find the ground state energy of the exciton we use the adiabatic approximation which allows us to decouple the fast particles motion in z-direction from their slow motion in the radial direction. The novel curves for the exciton ground state energy for different truncated pyramid heights, the base and upper radii are presented.

Introduction. Recently, the semiconductor self-assembled quantum dots (QDs) in a great variety of sizes and shapes with axial symmetry such as lens, disk or pyramids promising for future applications in micro- and opto-electronic devices are fabricated [1]. The binding energy of exciton in QDs increases sharply due to confinement and it is possible to observe them in the stable state up to room temperature The energy spectrum of exciton in QDs have been studied by using variational, diagonalization, finite element methods and others numerical procedures [2]. Different models of the confinement have been considered, exponential, Gaussian, parabolic, and hard wall with finite height [2]. Two-dimensional models which left to aside the effects related to the QDs thickness has been commonly used in these investigations. In this work we show that the confinement potential and the barrier height for the particles motion in the lateral direction in real QDs is very sensitive to the variation of the QD's profile and the thickness. To this end we calculate the ground state energy of exciton confined in QDs with truncated pyramid shape and different ratios of the upper and base radii, applying a simple variational procedure within framework of the adiabatic approximation [3].

Theory. To analyze the electronic spectrum in $In_{0.55}Ga_{0.45}As/Ga_{0.65}Al_{0.35}As$ QD which has the shape of a truncated quantum pyramid of the height d_0, the upper and base radii R_u and R_b, respectively ($R_u \leq R_b$), we consider a model [4] with conduction and valence band offsets, $V_e \approx 258meV$ and $V_h \approx 172meV$ (the labels *e* and *h* refer to the electron and to the hole parameters, respectively) and with the same physical parameters in the well and in the barrier corresponding to $In_{0.55}Al_{0.45}As$ structure: $\varepsilon = 12{,}71$, the effective masses, $m_e{*} = 0.076m_0$ and $m_h{*} = 0.45m_0$. The exciton effective Bohr radius, $a_0{*} = \hbar^2\varepsilon/\mu e^2 \approx 10.36nm$ and the exciton effective Rydberg, $Ry{*} = e^2/2\varepsilon a_0{*} \approx 5.47meV$ as the units of the length and the energy are used, being $\mu = m_e{*}m_h{*}/(m_e{*}+m_h{*}) \approx 0.065m_0$ the effective electron-hole reduced mass.

Typically, the InGaAs/GaAlAs pyramidal QDs have a ratio between height and radius much smaller than unity ($d_0 / R_b << 1$). This condition permits us to apply the adiabatic approximation and to separate the motions in *z* and in-plane directions [3]. As it is shown in the paper [4] the 3D problem for interacting particles in this case can accurately be approximated by a 2D problem in which the two-dimensional lateral confinement potential can be renormalized and be taken as $\widetilde{V}_i(\rho)=V_i$ for $\rho > R_b$ and $\widetilde{V}_i(\rho)=E_z(\rho,V_i)$ otherwise, where $E_z(\rho,V_i)$ is the energy of the lowest level in a quantum well with the barrier height V_i and the width equal to the pyramid thickness, $d(\rho)$ at a point whose distance from the axis is ρ . It is clear, that the smaller the pyramid thickness the lower are renormalized barrier heights for the electron and for the hole and the more sensitive is the shape of the lateral potential $\widetilde{V}_i(\rho)$ to a variation of the pyramid profile and the thickness. Therefore this model strictly speaking is not two-dimensional and it takes partially into account the effect of the transversal thickness and profile of an almost flat QDs. Below we describe how can be found the lowest energies of the electron, hole and, exciton in truncated pyramid.

Free particles motion in quantum pyramid. The ground state wave functions of the free electron and hole in quantum pyramid, $\phi_i(\boldsymbol{\rho}_i)$, $i = e,h$ are solution of the one-dimensional wave equation:

$$H_{0i}(\rho_i)\phi_i(\rho_i)=E_i\phi_i(\rho_i); \quad H_{0i}(\rho_i)=-\frac{\eta_i}{\rho_i}\frac{d}{d\rho_i}\rho_i\frac{d}{d\rho_i}+\widetilde{V}_i(\rho_i); \quad i=e,h; \qquad (1)$$

where $\eta_i=\mu/m_i^*$; $\widetilde{V}_i(\rho_i)=\widetilde{V}_i\,\vartheta(R-\rho_i)$. As the potential of these one-dimensional wave equations for electron and hole are piecewise constant, their exact solutions $\phi_e(\boldsymbol{\rho}_e)$ and $\phi_h(\boldsymbol{\rho}_h)$ can be found in an analytical form in terms of the cylindrical functions, meanwhile the ground state energies E_e .and E_h can be calculated by solving the corresponding transcendental equation. We assume that for exciton strongly confined in QD the adiabatic approximation can be used as a starting point for qualitative analysis of this complex due to the fact that the effective hole mass in $In_{0.55}Al_{0.45}As$ material is essentially greater than the effective mass of the electron and this difference is more relevant in conditions of the strong confinement as the hole motion becomes slower. The first step of the adiabatic approximation consists of the freezing of the hole motion and depreciating of the term of the hole kinetic energy. Under this consideration the exciton problem is reduced to an off-center donor, D^0 one.

Off-center donor D^0 in quantum pyramid. Being $\boldsymbol{\rho}_h$ the position vector of the ion and $\boldsymbol{\rho}_e$ the position vector of the electron, the dimensionless Hamiltonian and the wave equation for the donor D^0 can be written as

$$\begin{aligned} &H_{D^0}(\boldsymbol{\rho}_e,\boldsymbol{\rho}_h)=H_{0e}(\boldsymbol{\rho}_e)-2/|\boldsymbol{\rho}_e-\boldsymbol{\rho}_h|;\\ &H_{D^0}(\boldsymbol{\rho}_e,\boldsymbol{\rho}_h)\psi_{D^0}(\boldsymbol{\rho}_e,\boldsymbol{\rho}_h)=E_{D^0}(\boldsymbol{\rho}_h)\psi_{D^0}(\boldsymbol{\rho}_e,\boldsymbol{\rho}_h)\end{aligned} \qquad (2)$$

If we choose the trial function in the form;

$$\psi_{D^0}(\boldsymbol{\rho}_e,\boldsymbol{\rho}_h)=\phi_e(\boldsymbol{\rho}_e)\Phi(|\boldsymbol{\rho}_e-\boldsymbol{\rho}_h|) \qquad (3)$$

the following differential equation for the function $\Phi(\rho)$ can be obtained by using the fractal dimension method [5]:

$$-\frac{\eta_e}{J_0(\rho,\rho_h)}\frac{d}{d\rho}J_0(\rho,\rho_h)\frac{d\Phi(\rho)}{d\rho}-\frac{2}{\rho}\Phi(\rho)=\left[E_{D^0}(\rho_h)-E_e\right]\Phi(\rho) \qquad \text{(4a)}$$

where ρ_h is the distance of the ion position from the pyramid axis and the Jacobian, $J_0(\rho,\rho_h)$ is defined as:

$$J_0(\rho,\rho_h)=r\int_0^{2\pi}\phi_e{}^2\left(\sqrt{\rho_h^2+r^2+2r\rho_h\cos\varphi}\right)d\varphi \qquad \text{(4b)}$$

In order to find the donor energy dependence on the ion position $E_{D^0}(\rho_h)$, which is used afterwards for calculating the exciton energy, we solve the equation (4a) numerically by using the trigonometric sweep method [6].

Exciton in quantum pyramid. Following the adiabatic approximation standard procedure we seek the eigenfunction of the Hamiltonian (5) in the form:

$$\psi_X(\mathbf{\rho}_e,\mathbf{\rho}_h)=\psi_{D^0}(\mathbf{\rho}_e,\mathbf{\rho}_h)\phi_X(\rho_h) \qquad \text{(5)}$$

where $\phi_X(\rho_h)$ is a solution of the one-dimensional wave equation:

$$-\frac{\eta_h}{\rho_h}\frac{d}{d\rho_h}\rho_h\frac{d\phi_X(\rho_h)}{d\rho_h}+\left[\tilde{V}_h(\rho_h)+E_{D^0}(\rho_h)\right]\phi_X(\rho_h)=E_X\phi_X(\rho_h) \qquad \text{(6)}$$

To solve the eigenproblem (6) and find the exciton energy E_X we can use again the trigonometric sweep method.

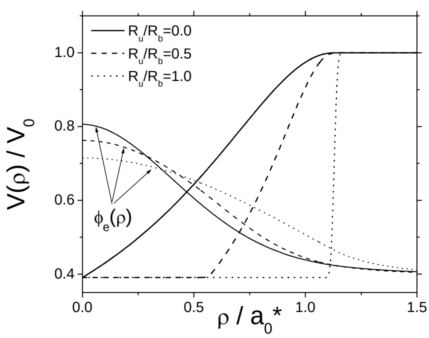

Fig.1. Confining potential shapes and corresponding wave functions for electron lateral motion in pyramid, truncated pyramid and disk.

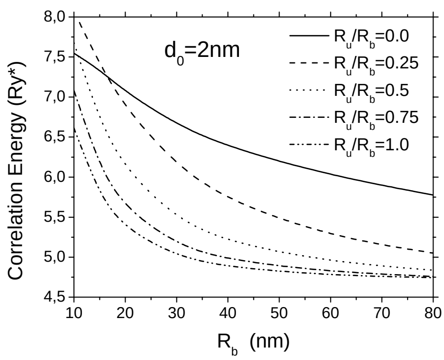

Fig.2. Exciton correlation energies as a function of the pyramid base radius for different ratios R_u / R_b.

In Fig. 2 and Fig. 3 we display the calculation results for the exciton correlation energies, $E_c(X)$ as a functions of the $In_{0.55}Ga_{0.45}As/Ga_{0.65}Al_{0.35}As$ quantum pyramid base radius, with different ratios R_u / R_b and pyramid heights defined as a difference between the energies of the

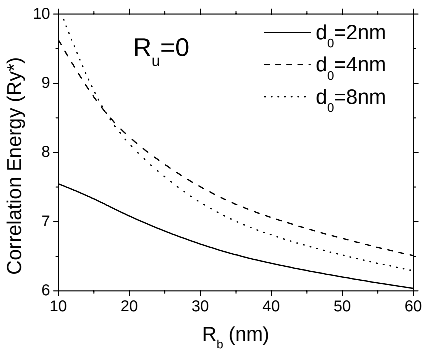

Fig 3. The exciton correlation energy in conical QD as a function of the quantum cone radius for three different cone heights.

electron-hole pair in the free and coupled states, $E_c(X) = E_e + E_h - E(X)$. It is seen from the Fig. 2 that correlation energies in pyramids with different ratios R_u / R_b decrease as the base radius increases and tends to the exact value of the 2D free exciton binding energy, 4Ry*. Additionally, it should be noted that the exciton correlation energy is strongly dependent of the QD morphology. Generally, the smaller R_u / R_b ratio, the stronger is the confinement in QD and the larger is exciton correlation energy. Therefore, the increase of the R_u / R_b ratio provides more rapid convergence the correlation energy to the free exciton 2D limit. One can see the crossover of the curves corresponding to the pyramid and the truncated pyramid with ratios 0.25 an 0.5 as the base radius tends to zero. It is due to the effect of the electron wave function leaking in the barrier region in pyramid, provided an increasing of the electron-hole separation. In Fig. 3 we compare the dependencies of the exciton correlation energies on the base radius in pyramids with different heights. Generally decreasing of the pyramid height provides the increase of the confinement and consequently the exciton correlation energy. The only crossover of the curves observed in Fig.3 is also due to the effect of the leaking of the electron wave function in the pyramid with smaller height

Acknowledgement This work was partially financed by the Universidad Industrial de Santander (UIS), through the General Researches (DIF) and the Colombian Agency COLCIENCIAS (Cod 1106-05-025-96). J. H. Marín wishes to thank the Universidad Nacional, Sede-Medellín for the permission to stay during his sabbatical year at the UIS.

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