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Exciton and biexciton binding and vertical Stark effect in a model lens-shaped quantum box: Application to InAs/InP quantum dots

C. Cornet *, J. Even, S. Loualiche

FOTON-UMR 6082 au CNRS, INSA de Rennes, 20 Avenue des Buttes de Coesmes, CS 14315, F-34043 Rennes Cedex, France

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Abstract

The problem of excitonic and biexcitonic binding is studied in the system of parabolic coordinates for a lens-shaped quantum box. The exciton wavefunction is expanded in terms of electron–hole configurations made from electron and hole single-particle states. Configuration interaction method and perturbative calculations are used to study the competition between confinement and correlation effects. Biexcitonic binding energy is calculated in the strong confinement regime and a comparison to the case of a spherical box is made. Absorption spectra with and without correlation effects are computed for InAs/InP quantum dots. Excitonic binding energy and enhancement factor are estimated to be equal to about 20 meV and 1.5, respectively. The excitonic absorption is finally studied in the presence of a uniform vertical electric field. A weak vertical Stark effect is predicted for lens-shaped quantum box described within this model.

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1. Introduction

Recent research developments were devoted to nano-structured semiconductor materials. Quantum dots (QDs) may improve properties as compared to semiconductor quantum wells (QWs) for high performance optoelectronic devices [1–4]. Most of the theoretically predicted properties of the QDs have been experimentally demonstrated in the InAs/GaAs system [5–7]. In order to reach 1.55 µm wavelength used in optical telecommunications, growth of InAs QDs on InP substrate has been investigated in our laboratory [8–10]. Using simple one-band effective mass models, we have succeeded in obtaining a first description of the electronic properties of these QDs [11]. More accurate theoretical study of the electronic properties of QDs may be performed with various theo-

* Corresponding author.
E-mail addresses: charles.cornet@ens.insa-rennes.fr (C. Cornet), jacky.even@insa-rennes.fr (J. Even).

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retical schemes providing that precise descriptions of the size, shape and composition are given as input [12–14]. In the case of InAs/InP QDs however, data from characterization experiments are scarce. In such a case effective mass calculations for highly symmetric shapes (two-dimensional boxes [15], spherical QDs [2,16], ellipsoidal QDs [17]) may give indications about the influence of quantum confinement and correlation effects. These approaches are based on the fact that analytical expressions are known for the single-particle states wavefunctions. We recently proposed to use parabolic coordinates to obtain analytical solutions for the single-particle states in perfectly asymmetric lens-shaped QDs [18]. This work was extended to describe quantum wires and quantum rings within the same formalism [19]. In this work, we will focus on the calculation of excitonic and biexcitonic binding in lens-shaped QDs. The single-particle analytical wavefunctions will be used both for a perturbative approach and the configuration interaction (CI) method. The linear absorption spectra for InAs/InP QDs with and without Coulomb interaction will be compared. Finally, the excitonic absorption will be studied in the presence of a uniform vertical electric field.

2. Single-particle states

In the presence of an infinite potential barrier, the Schrödinger equation is equivalent to the Helmholtz equation [18]. The parabolic set of coordinate sets may be used to reach separable solutions described in Helmholtz equations. The parabolic set of unitless coordinates (u, v, ϑ) is defined by a transformation of Cartesian coordinates ($0 \leqslant u \leqslant \infty$, $0 \leqslant v \leqslant \infty$ and $0 \leqslant \theta \leqslant 2\pi$): $x = auv\cos(\vartheta)$, $y = auv\sin(\vartheta)$ and $z = a(u^2 - v^2)/2$ (a is the parameter of the parabolic metric). Then, for an infinite potential barrier the Hamiltonian is

$$H = \frac{-\hbar^2}{2}\vec{\nabla}\frac{1}{m(\vec{r})}\vec{\nabla} = -\frac{\hbar^2}{2a^2(u^2+v^2)} \times \left[\frac{1}{u}\frac{\partial}{\partial u}\frac{u}{m_{(u,v)}}\frac{\partial}{\partial u} + \frac{1}{v}\frac{\partial}{\partial v}\frac{v}{m_{(u,v)}}\frac{\partial}{\partial v}\right] - \frac{\hbar^2}{2a^2u^2v^2m_{(u,v)}}\frac{\partial^2}{\partial\theta^2}.$$

In that case, the Hamiltonian is separable in u, v and ϑ coordinates and the single-particle wavefunction appears a product of functions of independent variables $\Xi(u, v, \theta) = f(u)g(v)e^{in\theta}$. The f and g functions are solutions of two coupled differential equations with a separation constant C

$$u^2\frac{d^2 f}{du^2} + u\frac{df}{du} + \left(Eu^4 - Cu^2 - n^2\right)f = 0$$

and

$$v^2\frac{d^2 g}{dv^2} + v\frac{dg}{dv} + \left(Ev^4 + Cv^2 - n^2\right)g = 0,$$

where $E = E_r/E_{\infty P}$ a dimensionless energy, E_r the actual energy and $E_{\infty P} = \frac{\hbar^2}{2ma^2}$ a unit energy adapted to the parabolic system of coordinates. Solutions of these equations [18], include confluent hypergeometric functions of first kind ϕ

$$f(u) = F(u, C, E, n) = \lambda_f e^{-i\sqrt{E}u^2/2}\left(i\sqrt{E}\,u^2\right)^{n/2} \times \phi\left(\frac{-iC}{4\sqrt{E}} + \frac{n+1}{2}, n+1, i\sqrt{E}u^2\right)$$

and

$$g(v) = F(v, -C, E, n) \quad (\lambda_f \text{ is a constant}).$$

A symmetric disk shape may be defined by the intersections of the two parabolas ($u = u_0 = 1$ and $v = v_0 = 1$) and rotated around the z axis (Fig. 1a). The height to diameter ratio (HDR) and volume V are equal respectively to 0.5 and $V = \pi a^3/2$. A relation between E and C is defined by the boundary conditions: $F(1, C, E, n) = 0$ [18]. If $C = 0$, the solutions of the problem contain simple $J_{n/2}(\sqrt{E}\,u^2/2)$ Bessel functions. This is in particular the case for the $1S$ ground state with $n = 0$ and $E = 23.1$. The solutions with $C \neq 0$ are twice degenerated: $\chi(u, v) = F(u, C, E, 0)^* F(v, -C, E, 0)$ and $\chi(u, v) = F(u, -C, E, 0)^* F(v, C, E, 0)$ with $E = 62.0$ and $C = 13.5$ correspond to the $2S$ state. Single-particle electronic states of a quantum box with flat bases (lens shape with HDR = 0.25 and $V = \pi a^3/4$) are readily obtained by keeping only odd solutions of the symmetric disk case with $C \neq 0$ [18]: $\chi(u, v) = F(u, C, E, 0)^* F(v, -C, E, 0) - F(u, -C, E, 0)^* F(v, C, E, 0)$. The $1S$ ground state of the lens-shaped QD corresponds to the $2S_u$ state of the disk-shaped QD