Comparison of electric field effects on carriers between spherical quantum dots and cylindrical quantum wires

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We investigate the effect of an electric field applied to two systems; a spherical quantum dot and a cylindrical quantum wire. In the latter system the field is applied perpendicular to the cylinder axis. We are interested on the energy ground state of carriers in the quantum dot and wire using an infinite confining potential well model. We perform a variational calculation for both systems and for low electric fields we find a quadratic shift of the energy levels with the electric field. For strong fields the Stark shift of the energy groundstate increases almost linearly with the electric field. In order to compare the results of both systems, we choose the radii of the sphere and the cylinder to be equal. For same radii the Stark shift of the sphere is smaller than that of the cylinder.

1 Introduction

In this paper, we present a theoretical calculation of the shift of the energy levels of carriers in spherical quantum dots (QD) and in cylindrical quantum wires (QW) with an electric field applied transverse to the axis of cylindrical symmetry. It is important to find the shift of the groundstate energy of the confined carriers in the transverse fields to be able to determine the binding energies of excitons and hydrogenic impurities in quantum wires in the same fields. There has been much work on the transverse Stark effect in quantum wells where an electric field is applied along the direction of confinement in the well [1–7]. However, to our knowledge little work has appeared concerning the Stark effect in QW when the Stark field is applied perpendicular to the wire axis. Dupertuis, et. al. [8] investigated the effect of an electric field on the energies of electrons in V shaped quantum wires but did not show what they used for the confining potential. The electric field in their case had components parallel and perpendicular to the V shaped wire. They found excited states with many nodes, which get split with the electric field. Huynh Thanh, et. al. [9] investigated the confined Stark effect in quantum wires with parabolic confinement and found a quadratic Stark effect at all electric fields. Benner and Haug [10] considered the Stark effect in quantum wires also assuming parabolic confinement. There has also been experimental work on the photoluminescence in quantum wires in an electric field. [11,12]. Arakawa, et. al. [11] found a blue shift in the photoluminescence due to excitons in quantum wires in the presence of an electric field. In their case, the quantum wires were V shaped. Rinaldi, et. al. [12] also observed a small blue shift, which they believed, was due to the piezoelectric field, caused by strain in the quantum wires. In spherical QD`s we

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must mention the works of Wen et al. [13], Chang and Xia [14] and Menéndez-Proupin and Trallero-Giner [15], in which the Stark effect on the energy levels of excitons in quantum dots (QD's), was investigated. In Ref. [14] the Stark effect was calculated for both single particle and exciton states with an infinite hard-wall confinement potential. A good survey on the physics, optical spectroscopy, and application-oriented research of semiconductor QD´s is given in Ref. [16]. Previous calculations similar to the present work on Stark effect of a single particle in a spherical QD are very few. Bose [17] used quantum perturbation theory to calculate the Stark effect on spherical quantum dots. Niculescu [18] used a variational procedure on the electronic states in a spherical QD's with parabolic confinement in two models: when this confinement is not limited and when it becomes constant outside a fixed value of the radius. He compared these results with those of his own variational calculations of spherical step-wise QD's and found that the parabolic potential leads to the smaller electric-field-induced shifts. Chang and Xia [14] calculated exactly the Stark effect in QD with an infinite hard-wall confinement potential. Here we present a variational calculation of the shift of the carriers ground state energy in QW``´s and spherical QD's using an infinite hard-wall confining potential. It is important to mention that this particular potential avoids the existence of quasibound states for strong fields, since a strong enough electric field (or applied over large regions) combined with finite confining potential will tend to eject the carrier from the bound state.

2   Theory

We describe a charged particle in a spherical QD (SQD) or in a cylindrical QW (CQW) in the presence of an electric field. For the QD the field is applied along the z-axis and for the cylinder (with its axis parallel to the z-axis) the electric field is applied along the x-axis. The Hamiltonians are:

$$H_{\text{SQD}} \; = \; \frac{p^2}{2m*} - qFr\cos\theta + V_{SQD}(r) \quad , \; H_{\text{CQW}} \; = \; \frac{p^2}{2m*} - qF\rho\cos\phi + V_{CQW}(\rho) \qquad (1)$$

where F is electric field, $m*$ and q are the carrier effective mass and charge respectively, r is the distance of the carrier from the center of the sphere, θ is the angle between the position vector of the carrier and the electric field direction. ρ is the distance of the carrier from the center of the cylinder, ϕ is the angle between the position vector of the carrier and the electric field direction. In both cases V are the confining potentials using the infinite well model which vanishes inside each structure defined by radius d and becomes infinite outside. Here, d has the same value for the sphere and for the cylinder. Our assumption of a constant electric field is based on a negligible difference between the dielectric constants of each structure and its surroundings. This would be the case for a GaAs structure embedded in $Ga_{1-x}Al_xAs$ surroundings. In the QD exact calculation of Ref. [14], the carrier wave function was expanded in the basis of the single-particle wave functions in the absence of electric fields. Therefore, in order to simplify these calculations, we chose as our variational wave function

$$\Psi_{SQD}(\mathbf{r}) \; = \; N_{SQD}j_0(k_{SQD}r)\exp(\beta_{SQD}r\cos\theta)$$

and analogously, for the cylinder we choose

$$\Psi_{CQW}(\mathbf{r}) \; = \; N_{CQW}J_0(k_{CQW}\rho)\exp(\beta_{CQW}\rho\cos\phi)\exp(ikz)$$

where the product $k_{SQD}d$ is the first zero of the spherical Bessel function $j_0(x)$ and the product $k_{CQW}d$ is the first zero of the Bessel function $J_0(x)$, β_{SQD} and β_{CQW} are the variational parameter which depend upon the electric field and N's are the normalization constants of the wave function. If q and F are positive then the particle will be pushed to positive values of z, and therefore both β are positive. The exponential factor in the variational wave functions is chosen in analogy to the trial wave functions used for electrons in an electric field in bulk semiconductors and semiconducting quantum wells, which seems to

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give good results for the ground state when compared to the exact wavefunctions involving Airy functions.

A simple calculation shows that the normalization constants are given by

$$N_{SQD}^{-2} = 2\pi M_{\text{SQD}} \quad , \qquad N_{CQW}^{-2} = 2\pi M_{\text{CQW}} \tag{3}$$

where

$$M_{\text{SQD}} = \frac{\pi^{3/2}}{2k_1\beta^{1/2}} \int_0^d dr\, r^{1/2} J_{1/2}^2(k_1 r) I_{1/2}(2\beta r) \tag{4}$$

$$M_{CQW} = 2\pi \int_0^d d\rho\, \rho J_0^2(k_1\rho) I_0(2\beta\rho) $$

Here $J_\nu(x)$ are Bessel functions and $I_\nu(x)$ are the modified Bessel functions of the first kind. A straightforward calculation yields the change in the carriers energy due to the electric field:

$$\Delta E_{\text{SQD}} = E_{SQD}(0) - E_{SQD}(\beta) = \frac{eF}{2}\frac{d}{d\beta}\ln(M_{SQD}) - \frac{\hbar^2\beta^2}{2m*} \tag{5}$$

$$\Delta E_{\text{CWQ}} = E_{CQW}(0) - E_{CQW}(\beta) = \frac{eF}{2}\frac{d}{d\beta}\ln(M_{CQW}) - \frac{\hbar^2\beta^2}{2m*} \tag{6}$$

3 Results

The expression for ΔE's as a function of β's are minimized to obtain a lower limit of ΔE's as a function of the structure radii and the electric field. In Fig. 1 the Stark shift of the carrier's energy $-\Delta E$ is shown as a function of the electric field for various radii d. This shift is given in electron Rydberg units where Ry=$(e^2/2\kappa a)$, the radii of both QD and QW are given in electron Bohr radii where $a = (h^2\kappa/m*e^2)$, the electric field is given in atomic units $F_0 = (e/\kappa a^2)$ and κ is the dielectric constant of the semiconductor. The results for the shift in the QD's are approximately one third of those in the QW's. The shift in the QD's are smaller because the average carrier density probability is smaller in the QD when the field pushes the carrier to lower energies. Geometrically this means that the concavity of the sphere is stronger than in the cylinder, that is, as a function of the coordinate along the cylinder axis, the QW boundary does not change. ΔE is a nonlinear function of the electric field for low electric fields and an approximately linear function of the electric field for higher electric fields. For the QD our results agree quite well with those of Ref. [14]. It can be shown that the slope of the linear shift increases with increasing radii. These results show that the presence of the electric field decreases the energy of the carriers in the structures below their value in the absence of the electric field. Furthermore, we have also compared the results of an exact calculation of the Stark effect in cylindrical QD's [19] with our variational results and the agreement is very good.

We can also point out a common fact which has been often overlooked. This consists of the existence of quasi-bound states (instead of bound states), if the electric field is strong enough and it is applied over a distance larger than the QD radius. For example, there exist calculation models in quantum wells [20] and quantum wires [21] which assume a potential term in the Hamiltonian qFz for all z, in which the authors fail to notice or to mention that they are dealing with quasi-bound states.

In summary, we presented very simple one-parameter analytical expressions that yielded, after minimization, very good results when compared with more complicated and exact results, as those given in Ref. [14] for QD and Ref. [19] for QW.
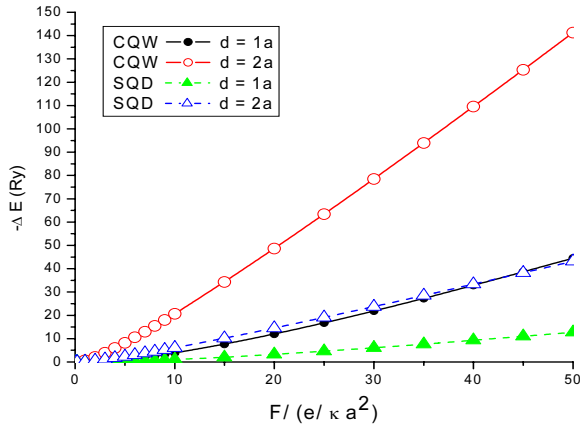

Fig. 1   The Stark shift of the carrier's energy $-\Delta E$ is shown as a function of the electric field for various radii d. In this figure the quantities are given in atomic units appropriate for the electron in the semiconductor. CQW indicates cylindrical quantum wire and SQD indicates spherical quantum dot.

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