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Exact analytical solutions for shallow impurity states in symmetrical paraboloidal and hemiparaboloidal quantum dots

Research Article

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Abstract: The problem of a shallow donor impurity located at the centre of a symmetrical paraboloidal quantum dot (SPQD) is solved exactly. The Schrödinger equation is separated in the paraboloidal coordinate system. Three different cases are discussed for the radial-like equations. For a bound donor, the energy is negative and the solutions are described by Whittaker functions. For a non-bound donor, the energy is positive and the solutions become coulomb wave functions. In the last case, the energy is equal to zero and the solutions reduce to Bessel functions. Using the boundary conditions at the dot surfaces, the variations of the donor kinetic and potential energies versus the size of the dot are obtained. The problem of a shallow donor impurity in a Hemiparaboloidal Quantum dot (HPQD) is also studied. It is shown that the wave functions of a HPQD are specific linear combinations of those of a SPQD.

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Keywords: paraboloidal quantum dot • hemiparaboloidal quantum dot • donor impurity

1. Introduction

During the last two decades, semiconductor quantum dots (QD's) have attracted great interest thanks to their remarkable electronic and optical properties [1–3]. Indeed, due to the three dimensional confinement, the charge carriers in a single QD are spatially localized and their energy levels are quantized. The overlap between the charge carriers wave functions is increased. As a consequence, the recombination probability of electrons and holes is raised. The oscillator strength of interband optical transitions concentrated only on discrete states is more important. Semiconductor QD's behave like artificial atoms. Their properties are promising in the improvement of existing electronic and photonic [4, 5] devices, and in the development of novel device concepts such as the single

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electron transistor [6]. Unfortunately, with the physical [7–9] and chemical [10, 11] growth techniques used to fabricate QD's, it has been very difficult to grow nanometre scale QD's with a uniform size. Moreover, the density of QD's produced was very low and it was very difficult to stack several dots in a small active region. In the past several years, new technologies for fabricating QD's have emerged, namely the self-organization or self-assembling growth techniques such as the Stranski-Krastanow (SK) mode and atomic layer epitaxy (ALE) [5]. With these techniques, the scientists can, at present, fabricate nanometre scale QD's with good quality, reduced size fluctuations and high density. The QD's obtained by ALE are similar to symmetrical paraboloidal quantum dots, those obtained by the SK mode look like hemiparaboloidal quantum dots, this is the first reason for the choice of the geometries studied in the present article.

Using the effective mass approximation and describing the confinement by an infinite barrier, some pioneering theoretical works have obtained analytic or semi-analytic solutions for single particles (electron or hole) or quasi-particles (neutral donor or exciton) in spheres [12], cones [13], rectangles [14], discs [15], cylinders [15], domes and lenses [16, 17]. The present article is also motivated by recent works where appropriate orthogonal curvilinear coordinate systems are used in order to solve the quantum dot problems exactly. Indeed, van den Broek and Peeters [18] used the elliptic coordinate system in two dimensions to solve the single particle problem in an elliptical dot. Cantele et al. [19, 20] used the spheroidal coordinate system to solve the single particle problem in oblate and prolate spheroidal quantum dots. Even and Loualiche [21] used the parabolic coordinate system to determine the energy levels and the wave functions of an electron in a lens shaped quantum dot. Yang and Huang [22] used the parabolic coordinate system to calculate the energy spectrum of a hydrogen impurity located in the centre of a parabolic quantum dot. In the present work, we focus on the problem of a hydrogenic donor impurity placed at the centre of a symmetrical paraboloidal quantum dot (SPQD). We express the donor Hamiltonian in the paraboloidal coordinate system[1,2] [23]. We show that the Schrödinger equation is separated into two radial-like coupled equations and one angular-like equation. The presence of coupling constants makes the resolution more difficult than in standard problems where only the application of the boundary conditions leads to the particle energies. In the light of these elements, we solve the radial-like equations exactly and determine the energy and the coupling constants versus the dot size. Finally, we treat the problem of a hydrogenic donor impurity placed at the centre of a hemiparaboloidal quantum dot (HPQD). We show that the ground state of a HPQD is identical to the fourth excited state of the SPQD.

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2. Theory

2.1. Dots description

The paraboloidal quantum dot (PQD) is a quantum box which may be obtained by the intersection of the paraboloids whose equations are given by:

$$\sqrt{(x^2+y^2+z^2)}+z=\xi_0 \qquad \text{and}$$
$$\sqrt{(x^2+y^2+z^2)}-z=\eta_0 \tag{1}$$

ξ_0 and η_0 are two positive constants. The PQD is similar to a biconvex lens with two different curvatures. Its common physical parameters are the thickness at the centre T, the circumference radius R and the volume V:

$$T=\frac{(\xi_0+\eta_0)}{2}, \quad R=\sqrt{\xi_0\eta_0}, \quad V=\frac{\pi}{2}R^2T. \tag{2}$$

In the particular case of a SPQD, ξ_0 is equal to η_0 (see figure 1a). The dot parameters reduce to:

$$T=\xi_0, \quad R=\xi_0, \quad V=\frac{\pi}{2}\xi_0^3. \tag{3}$$

The hemiparaboloidal quantum dot (HPQD) is defined by the space region which corresponds to $z \geq 0$ in the SPQD (see figure 1b). It is similar to a dome or a plano-convex lens. Its physical parameters are:

$$T=\frac{\xi_0}{2}, \quad R=\xi_0, \quad V=\frac{\pi}{4}\xi_0^3. \tag{4}$$

2.2. Paraboloidal coordinate system

Owing to the geometry of the dots considered in this article, it is more suitable to work in the paraboloidal coordinate system[1,2] [23]. The set of paraboloidal coordinates (ξ, η, φ) used in this work is defined by the following transformation to Cartesian coordinates:

$$x=\sqrt{\xi\eta}\cos(\varphi), \quad y=\sqrt{\xi\eta}\sin(\varphi) \quad \text{and} \quad z=(\xi-\eta)/2 \tag{5}$$

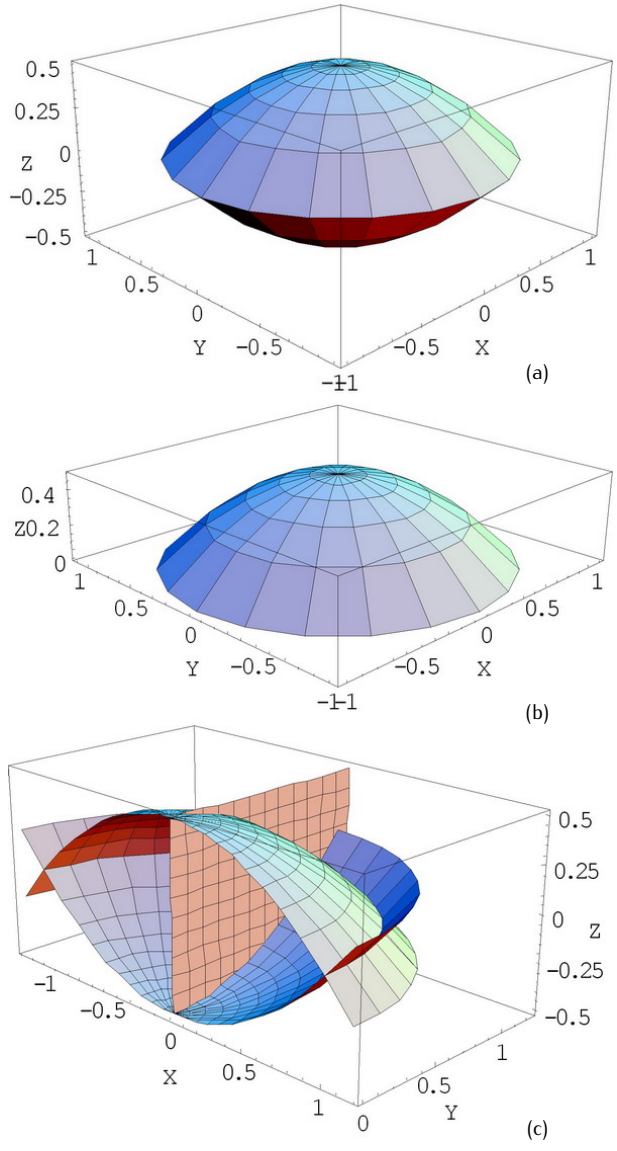

Figure 1. Representations of the symmetrical paraboloidal quantum dot (a), the hemiparaboloidal quantum dot (b) and the paraboloidal coordinate system (c). In figure 1c, the paraboloids correspond to $\xi_0 = 1$ and $\eta_0 = 1$, the vertical plane corresponds to $\varphi = \pi/2$.

where:

$$0 \leq \xi \leq \infty,\ 0 \leq \eta \leq \infty \ \text{ and } \ 0 \leq \varphi \leq 2\pi. \tag{6}$$

The inverse transformation from the Cartesian coordinates is:

$$\xi = \sqrt{(x^2+y^2+z^2)} + z, \quad \eta = \sqrt{(x^2+y^2+z^2)} - z \quad \text{and} \quad \varphi = \arctan\frac{y}{x}. \tag{7}$$

Figure 1c gives the two paraboloids corresponding to $\xi = 1$, $\eta = 1$ and the vertical plane corresponding to $\varphi = 1$.

2.3. Schrödinger equation

Let us consider an electron (e) revolving round an ionized hydrogenic donor impurity (D^+), placed at the centre of a SPQD. We assume that the electron is completely confined in the SPQD by an infinite potential barrier. We neglect the effect of the polarization charges induced at the surface of the dot. In the framework of the effective mass approximation and assuming isotropic parabolic and non degenerated bands, the Schrödinger equation for the donor wave function $\psi(x,y,z)$ is:

$$-\frac{\hbar^2}{2m^*}\nabla^2\psi(x,y,z) + \left[-E_{D^0} - \frac{e^2}{\varepsilon\sqrt{(x^2+y^2+z^2)}} + V(x,y,z)\right]\psi(x,y,z) = 0. \tag{8}$$

E_{D^0} is the donor energy. m^* is the electron effective mass. ε is the dot dielectric constant. $V(x,y,z)$ is the confinement potential, it is equal to zero and infinity respectively inside and outside the dot. Afterwards, we use as the unit of length the $3D$ donor effective Bohr radius: $a_{3D} = \varepsilon\hbar^2/e^2m^*$, and as the unit of energy: $E_{3D} = \hbar^2/2m^*a_{3D}^2$ which represents the absolute value of the $3D$ donor ground state energy. Thus, the Schrödinger equation reads:

$$\nabla^2\psi(x,y,z) + 2\left[E + \frac{1}{\sqrt{(x^2+y^2+z^2)}} - V(x,y,z)\right]\psi(x,y,z) = 0. \tag{9}$$

$E = E_{D^0}/2E_{3D}$ is the donor dimensionless energy.
In the paraboloidal coordinate system, the Schrödinger equation becomes :

$$\nabla^2\psi(\xi,\eta,\varphi) + 2\left[E + \frac{2}{(\xi+\eta)} - V(\xi,\eta)\right]\psi(\xi,\eta,\varphi) = 0. \tag{10}$$

2.4. Exact solutions

In the case of a finite potential barrier, the operator $V(\xi,\eta)$ describing the confinement inside the dot is not separable, in contrast to what has been asserted in reference [22]. As a consequence, the donor Hamiltonian is only separable in (ξ,η) and φ coordinates, and $\psi(\xi,\eta,\varphi) = h(\xi,\eta)\exp(im\varphi)$ is the simplest expression of the eigenfunction. m is an integer such as $m\hbar$ is an eigenvalue of the operator L_z.

However, in the case of an infinite potential barrier, the operator $V(\xi,\eta)$ may be expressed in the form: $V_1(\xi)+V_2(\eta)$. So, the donor Hamiltonian is fully separable and the wave function may be written as a product of the functions of independent variables: $\psi(\xi,\eta,\varphi)=f(\xi)\,g(\eta)\exp(im\varphi)$. The functions f and g are solutions of the two coupled differential equations:

$$\frac{d}{d\xi}\left(\xi\frac{df}{d\xi}\right)+\left[\frac{E}{2}\xi-\frac{m^2}{4\xi}+\beta\right]f=0, \tag{11}$$

$$\frac{d}{d\eta}\left(\eta\frac{dg}{d\eta}\right)+\left[\frac{E}{2}\eta-\frac{m^2}{4\eta}+\gamma\right]g=0. \tag{12}$$

β and γ are two separation constants defined by the following equation:

$$\beta+\gamma=1. \tag{13}$$

We begin by the resolution of equation (11). We first consider the case where the donor dimensionless energy E is negative, we set: $E=-1/2\lambda^2$ and $\xi=\lambda\rho$. The equation (11) becomes:

$$\frac{d^2f}{d\rho^2}+\frac{1}{\rho}\frac{df}{d\rho}+\left[-\frac{1}{4}-\frac{m^2}{4\rho^2}+\frac{\beta\lambda}{\rho}\right]f=0. \tag{14}$$

If we write $f(\rho)=u(\rho)/\rho^{1/2}$, equation (14) reduces to:

$$\frac{d^2u}{d\rho^2}+\left[-\frac{1}{4}+\frac{\beta\lambda}{\rho}+\frac{\left(1/4-(m/2)^2\right)}{\rho^2}\right]u=0. \tag{15}$$

Equation (15) is the Whittaker's differential equation whose solutions read [24]:

$$u(\rho)=\exp\left(-\frac{\rho}{2}\right)\rho^{(|m|+1)/2} \cdot M\left(\frac{1}{2}+\frac{|m|}{2}-\beta\lambda\,,1+|m|\,,\rho\right) \tag{16}$$

M is the Kummer's confluent hypergeometric function [24]. Hence, $f(\xi)$ is:

$$f(\xi)=\exp\left(-\frac{\xi}{2\lambda}\right)\left(\frac{\xi}{\lambda}\right)^{|m|/2} \cdot M\left(\frac{1}{2}+\frac{|m|}{2}-\beta\lambda\,,1+|m|\,,\frac{\xi}{\lambda}\right). \tag{17}$$

The resolution of equation (12) is similar to that of equation (11). It may be achieved following the steps detailed above. So, $g(\eta)$ is:

$$g(\eta)=\exp\left(-\frac{\eta}{2\lambda}\right)\left(\frac{\eta}{\lambda}\right)^{|m|/2} \cdot M\left(\frac{1}{2}+\frac{|m|}{2}-\gamma\lambda\,,1+|m|\,,\frac{\eta}{\lambda}\right). \tag{18}$$

The constant λ is determined from the boundary conditions $f(\xi_0)=0$ and $g(\eta_0)=0$ which are equivalent to the conditions:

$$M\left(\frac{1}{2}+\frac{|m|}{2}-\beta\lambda\,,1+|m|\,,\frac{\xi_0}{\lambda}\right)=0 \quad \text{and}$$
$$M\left(\frac{1}{2}+\frac{|m|}{2}-\gamma\lambda\,,1+|m|\,,\frac{\eta_0}{\lambda}\right)=0. \tag{19}$$

As a consequence, the donor energy E_{D^0} reads:

$$E_{D^0}=-\frac{m^*e^4}{2\lambda^2\varepsilon^2\hbar^2}. \tag{20}$$

When ξ_0 tends to infinity, λ tends to the principal quantum number n_{3D} $(n_{3D}\geq 1)$. The energy E tends to the limiting value $-1/2n_{3D}^2$. The wave functions given by equations (17) and (18) converge at infinity if and only if [24]:

$$\frac{1}{2}+\frac{|m|}{2}-\beta_{3D}n_{3D}=-n_1 \quad \text{and}$$
$$\frac{1}{2}+\frac{|m|}{2}-\gamma_{3D}n_{3D}=-n_2, \tag{21}$$

n_1 and n_2 are the parabolic quantum numbers defining the donor state in bulk semiconductor ($n_1\geq 0$, $n_2\geq 0$) [24]. Thus, the limiting values β_{3D} and γ_{3D} are:

$$\beta_{3D}=\frac{n_1}{n_{3D}}+\frac{1}{2n_{3D}}+\frac{|m|}{2n_{3D}} \quad \text{and}$$
$$\gamma_{3D}=\frac{n_2}{n_{3D}}+\frac{1}{2n_{3D}}+\frac{|m|}{2n_{3D}}. \tag{22}$$

In the second case, the donor dimensionless energy E is positive. So, we set: $E=1/2\mu^2$ and $\xi=\mu\rho$. The equation (11) becomes:

$$\frac{d^2f}{d\rho^2}+\frac{1}{\rho}\frac{df}{d\rho}+\left[\frac{1}{4}-\frac{m^2}{4\rho^2}+\frac{\beta\mu}{\rho}\right]f=0. \tag{23}$$

If we write $f(\rho)=u(\rho)/\rho^{1/2}$, equation (23) leads to:

$$\frac{d^2u}{d\rho^2}+\left[\frac{1}{4}+\frac{\beta\mu}{\rho}+\frac{\left(1-m^2\right)}{4\rho^2}\right]u=0. \tag{24}$$

We further set $\rho=2r$, then equation (24) gives:

$$\frac{d^2u}{dr^2}+\left[1+\frac{2\beta\mu}{r}+\frac{\left(1-m^2\right)}{4r^2}\right]u=0. \tag{25}$$

Equation (25) is a Coulomb differential equation whose regular solutions at $r = 0$ are [24]:

$$u(r) = C_m(\beta\mu)\, r^{(|m|+1)/2} \exp(-ir) \cdot M\left(\frac{|m|+1}{2} + i\beta\mu, |m|+1, 2ir\right). \quad (26)$$

Hence, $f(\xi)$ can be expressed as:

$$f(\xi) = C_m(\beta\mu)\left(\frac{1}{2^{(|m|+1)/2}}\right)\left(\frac{\xi}{\mu}\right)^{|m|/2} \exp\left(-i\frac{\xi}{2\mu}\right) \cdot M\left(\frac{|m|+1}{2} + i\beta\mu, |m|+1, i\frac{\xi}{\mu}\right). \quad (27)$$

The resolution of equation (12) in this case leads to the following expression of the function $g(\eta)$:

$$g(\eta) = C_m(\gamma\mu)\left(\frac{1}{2^{(|m|+1)/2}}\right)\left(\frac{\eta}{\mu}\right)^{|m|/2} \exp\left(-i\frac{\eta}{2\mu}\right) \cdot M\left(\frac{|m|+1}{2} + i\gamma\mu, |m|+1, i\frac{\eta}{\mu}\right). \quad (28)$$

The constant μ is determined from the continuity conditions at the surfaces of the dot $f(\xi_0) = 0$ and $g(\eta_0) = 0$ which are equivalent to the conditions:

$$M\left(\frac{|m|+1}{2} + i\beta\mu, |m|+1, i\frac{\xi_0}{\mu}\right) = 0 \quad \text{and} \quad M\left(\frac{|m|+1}{2} + i\gamma\mu, |m|+1, i\frac{\eta_0}{\mu}\right) = 0. \quad (29)$$

As a consequence, the donor energy E_{D^0} is:

$$E_{D^0} = \frac{m^* e^4}{2\mu^2\varepsilon^2\hbar^2}. \quad (30)$$

In the last case, the donor dimensionless energy E is equal to zero. If we let $\xi = \rho^2/4\beta$, equation (11) reduces to:

$$\rho^2\frac{d^2f}{d\rho^2} + \rho\frac{df}{d\rho} + \left[\rho^2 - m^2\right]f = 0. \quad (31)$$

Equation (31) is the modified Bessel differential equation whose regular solutions at $r = 0$ are [24]:

$$f(\rho) = C_m(\beta)J_m(\rho). \quad (32)$$

Thus, $f(\xi)$ can be written as:

$$f(\xi) = C_m(\beta)J_m\left(2\sqrt{(\beta\xi)}.\right) \quad (33)$$

In this case $g(\eta)$ is obtained by substituting ξ by η and β by γ in equation (33):

$$g(\eta) = C_m(\gamma)J_m\left(2\sqrt{(\gamma\eta)}.\right) \quad (34)$$

The critical dot size corresponding to a donor energy E_{D^0} equal to zero is determined from the boundary conditions $f(\xi_0) = 0$ and $g(\eta_0) = 0$. These equalities are equivalent to the conditions:

$$J_m\left(2\sqrt{(\beta\xi_0)}\right) = 0 \quad \text{and} \quad J_m\left(2\sqrt{(\gamma\eta_0)}\right) = 0. \quad (35)$$

2.5. Eigensolutions properties

Due to the symmetry of the SPQD (see figure 1a), it is important to discuss the symmetry of the wave functions $f_{m,\beta}(\lambda,\xi)\, g_{m,\gamma}(\lambda,\eta)\exp(im\varphi)$ with regard to the z-axis and to the plane $z = 0$. The rotational symmetry around the z-axis is governed by the integer m. Indeed, for even values of m we have:

$$\psi(\xi,\eta,\varphi) = \psi(\xi,\eta,\varphi+\pi). \quad (36)$$

And, for odd values of m we have:

$$\psi(\xi,\eta,\varphi) = -\psi(\xi,\eta,\varphi+\pi). \quad (37)$$

The reflection symmetry of the wave functions $f_{m,\beta}(\lambda,\xi)\, g_{m,\gamma}(\lambda,\eta)\exp(im\varphi)$ with respect to the plane $z = 0$ is determined by the constants β and γ. If $\beta = \gamma = 1/2$, the probabilities of finding the electron in the regions $z > 0$ and $z < 0$ are the same. So we can write:

$$\psi(\xi,\eta,\varphi) = \psi(\eta,\xi,\varphi). \quad (38)$$

If $\beta \neq 1/2$, then $\gamma = (1-\beta) \neq 1/2$. The reflection symmetry with respect to the plane $z = 0$ is broken. Nevertheless, it is possible to construct acceptable wave functions, from the symmetry point of view, by making the following linear combinations:

$$\psi^{\pm}(\xi,\eta,\varphi) = \exp(im\varphi) \cdot \left(f_{m,\beta}(\lambda,\xi)g_{m,\gamma}(\lambda,\eta) \pm (-1)^m f_{m,\beta}(\lambda,\eta)g_{m,\gamma}(\lambda,\xi)\right). \quad (39)$$

$\psi^+(\xi,\eta,\varphi)$ corresponds to the even solution while $\psi^-(\xi,\eta,\varphi)$ corresponds to the odd solution. The latter solution is particularly interesting because it leads to a vanishing wave function $\psi(\xi,\eta,\varphi)$ at the plane $z = 0$:

$$\psi^-(\xi,\eta,\varphi) = -\psi^-(\eta,\xi,\varphi). \quad (40)$$

As a consequence, $\psi^{-}(\xi,\eta,\varphi)$ may be a natural solution of the hydrogenic donor in HPQD (see figure 1b). In order to determine the wave functions in (39), we first specify m. For each value of the energy λ, we numerically look for β and γ associated with solutions satisfying $f_{m,\beta}(\xi_0)=0$ and $g_{m,\gamma}(\eta_0)=0$. The difficulty of this task, with regard to previous work [17, 21, 25] lies in the fact that for the same eigenstate $\psi^{+}(\xi,\eta,\varphi)$ or $\psi^{-}(\xi,\eta,\varphi)$, each value of the dot size ξ_0 corresponds to specific values of β and γ.

Finally, it is important to point out that for given values of m and β, equations (19), (29) and (35) may have more than one solution. If this is the case, the first solution will correspond to a quantum number $n=1$, the second solution will correspond to $n=2$ and so on until the last solution. In this way, the donor ground state is labelled: $(n=1, m=0, \beta=1/2)$, and it is associated with the ground state energy $E_{(1,0,1/2)}$. The first and second excited states are: $(n=1, m=\pm1, \beta=1/2)$, they belong to the same energy $E_{(1,1,1/2)}$. The third and fourth excited states are :$\{(n=1, m=0, \beta\to 3/4)\pm(n=1, m=0, \gamma\to 1/4)\}$ as defined in (39), they correspond to the energy $E_{(1,0,3/4)}$.

3. Results and discussions

We have determined the wave functions corresponding to the ground state $(n=1, m=0, \beta=1/2)$ and the two first excited states $(n=1, m=\pm1, \beta=1/2)$ of the neutral donor. We have also determined the wave functions corresponding to the third excited state $(n=1, m=0, \beta\to 3/4)$ and the fourth excited state $(n=1, m=0, \gamma\to 1/4)$ of the donor. Figures 2a and 2b show the charge distributions respectively of the states $(1,0,3/4)$ and $(1,0,1/4)$ as a function of x and z for a SPQD with a size $\xi_0=18.69$ at. units. The figures show a cross section through the neutral donor in the plane xOz, the nucleus being at the centre of the coordinate system. The charge density means the charge at the top of the vector $\mathbf{r}\equiv(r,\theta,\varphi)$. We can easily remark that for the states $(1,0,3/4)$ and $(1,0,1/4)$ there is a symmetry with regard to the rotation of π around the z-axis. On the other hand, there is a strong concentration of the charge towards respectively positive and negative values of z. So, we construct, as indicated in paragraph (2.5), even state $\psi^{+}=\{(1,0,3/4)+(1,0,1/4)\}/\sqrt{2}$ (see figure 2c) and odd state $\psi^{-}=\{(1,0,3/4)-(1,0,1/4)\}/\sqrt{2}$ (see figure 2d). We can note that in the state ψ^{-}, the probability of finding the electron at $z=0$ is equal to 0. As a consequence, ψ^{-} corresponds to the ground state of the HPQD.

We have numerically calculated the kinetic, potential and total energies of the neutral donor as a function of the dot parameter ξ_0 in the states $(1,0,1/2)$, $(1,\pm1,1/2)$ and

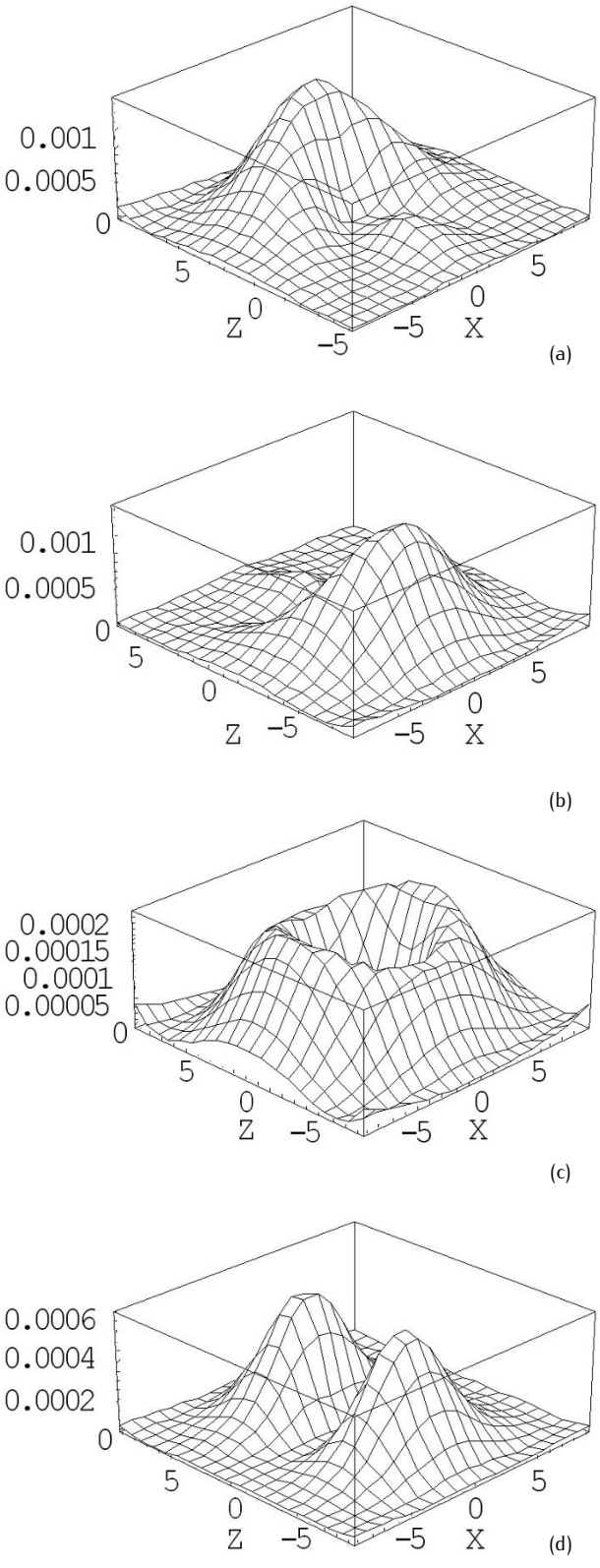

Figure 2. Charge distribution $r^2|\psi|^2$ as a function of x and z for the states (1,0,3/4) (a), (1,0,1/4) (b), $\{$ (1,0,3/4)+(1,0,1/4)$\}/\sqrt{2}$ (c) and $\{(1,0,3/4)-(1,0,1/4)\}/\sqrt{2}$ (d).

$\{(1,0,3/4) \pm (1,0,1/4)\}/\sqrt{2}$. Figure 3a shows the variations of kinetic energy T, potential energy V, total energy E and correlation energy $E_c = E - E_e$ of the neutral donor D^0 as a function of the dot size ξ_0 for the ground state $(1,0,1/2)$. E_e is the confined single electron energy without coulombic attraction i.e. in the state $1S_e$ [21]. When ξ_0 tends to infinity, T tends to 1/2, V tends to -1, E tends to $-1/2$ and E_c tends to $-1/2$. We recover perfectly the bulk situation. For a large size dot, the coulomb potential energy is predominant in comparison with the kinetic energy. So the total energy is negative $\left(E = -(1+2\exp(-\xi_0))^{-2}/2\right)$. When the dot size ξ_0 decreases, the effect of the volume reduction leads to an enhancement of the kinetic energy and to a small diminution of the coulomb potential energy. As a consequence, the donor energy increases. For a critical value of the dot size equal to $2.89\,at.units$, the donor energy is equal to zero. For a small size dot, the kinetic energy increases drastically like $11.56/\xi_0^2$, the coulomb potential energy varies like $-3.51/\xi_0$. The donor energy is close to the energy of a confined single electron in its ground state $1S_e$ [21].

Figure 3c presents the variations of kinetic energy T, potential energy V, total energy E and correlation energy E_c of the neutral donor versus the dot size ξ_0 for the third and fourth excited states $\{(1,0,3/4) \pm (1,0,1/4)\}/\sqrt{2}$. When ξ_0 tends to infinity, T tends to 1/8, V tends to $-1/4$, E tends to $-1/8$ and E_c tends to $-1/8$ in perfect agreement with bulk and semi-infinite semiconductor limits [26]. For a weak confinement, the coulomb potential energy dominates at the detriment of the kinetic energy. As a consequence, the total energy is negative $\left(E = -(1+\exp(-\xi_0))^{-2}/8\right)$. For a critical value of the dot size equal to $9.06\,at.units$, the kinetic and coulomb potential energies compensate each other. Thus, the donor energy is equal to zero. For a strong confinement, the kinetic energy increases rapidly like $31/\xi_0^2$, the coulomb potential energy decreases like $-3.12/\xi_0$. The donor energy is close to the energy of a confined single electron in its third and fourth excited states $2S_e$ and $1S_o$ [21].

4. Conclusion

The problem of a hydrogenic donor impurity confined in a Symmetrical Paraboloidal Quantum Dot (SPQD) was studied. The effective mass Hamiltonian and the Schrödinger equation in the paraboloidal coordinate system were derived. In the case of an infinite potential barrier, it was shown that the problem is entirely separated. The exact solutions of radial-like equations are Whittaker's functions for a bound donor, Coulomb func-

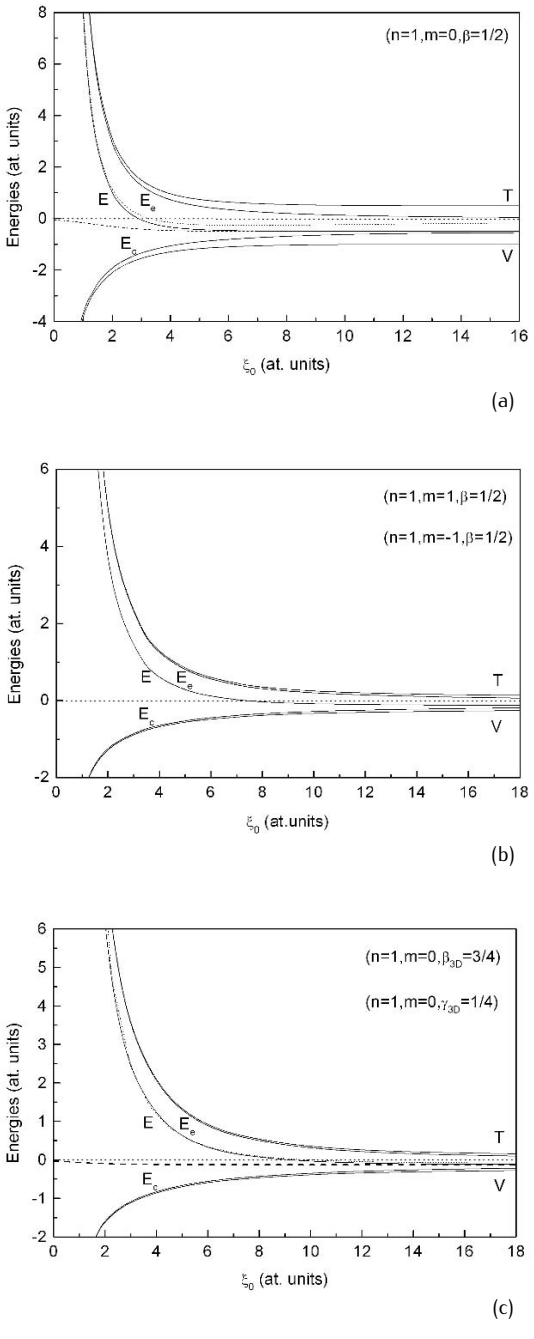

Figure 3. Total energy E, kinetic energy T, single electron energy E_e, Coulomb potential energy V and correlation energy $E_c = E - E_e$ versus the dot size ξ_0 for the states $(1,0,1/2)$ (a), $(1,\pm1,1/2)$ (b) and $\{(1,0,3/4) \pm (1,0,1/4)\}/\sqrt{2}$ (c). The dashed and dotted lines in (a) and (c) give the asymptotic behaviour of the energy E respectively for $\xi_0 \to \infty$ and $\xi_0 \to 0$.

tions for a non-bound donor and Bessel functions for a zero-energy donor. Using the boundary conditions at the dot surfaces, the variations of the donor energy were determined versus the dot size. The problem of a hydrogenic donor impurity in a Hemiparaboloidal Quantum dot (HPQD) was also investigated. Relying on the symmetry of the dot, it was shown that the ground state of a HPQD coincides with the fourth excited state of a SPQD. The geometries studied in this article are interesting indeed, they describe well the new kind of quantum dots such as domes [16], lenses [17] and rings [27]. The exact analytical solutions found may be used in the study of intrinsic and extrinsic effects such as: exciton, polaron, Stark effect and Zeeman effect, which will be the subject of forthcoming articles.

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