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# Spherically Bounded States of a Spherical Quantum Dot

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## *Abstract*

***The spherical bound states of a spherical quantum dot (QD) are calculated for the GaAs-$Al_xGa_{1-x}As$ system. The radial eigenfunction describing the electron motion, shows that the radius (r) of the spherical bound state when the azimuthal quantum number l equals zero, obey the relation r α $n^2$, where n is the principal quantum number. An expression for the maximum possible spherical bound state is therefore given and it is dependent on the radius of the QD.***

## 1.0 Introduction

Quantum structures such as a quantum dot have attracted much attention[1-7]. It's apparent zero dimensionality is as a result of confinement electrons in a space of the order of the de Broglie wavelength of the electron in all three directions. This causes the motion of the electron in the confinement to be completely quantized and only discrete bound electronic states are formed which correspond to the levels for an isolated atom[2] . Hence, a QD is sometimes called super atom. Considering a GaAs spherical QD in AlGaAs matrix, the eigenfunction of Schrodinger's equation (using the effective mass approximation) for the system is the product of a radial and an angular part. Assuming a spherically symmetric potential and focusing on the radial part a description of the motion of an election can be shown by the Legendre function[10,11]. In this paper the election bound states of a QD assuming spherical shape, is specified by the azimuthal quantum number,l =0 and confining effective potential V (with n= 1,2,3 …..), is considered.n being the principal quantum number.

The rest of the paper is organized as follows. In section 2, we present the theoretical formalism restricting our focus to l = 0. Section 3, covers an application and conclusions.

## 2.0 Theoretical formalism.

The schrodinger wave equation describing the electron motion is

$$H\Psi = E\Psi \tag{1}$$

In spherical polar coordinates this becomes

$$\left\{-\frac{\hbar^2}{2m}\frac{1}{r^2}\left[\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)-L^2\right]+V(r)\right\}\psi_{nlm}=E\psi_{nlm} \tag{2}$$

$$where\, L^2=\frac{1}{Sin\,\theta}\frac{\partial}{\partial\theta}\left(Sin\,\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{Sin^2\theta}\frac{\partial^2}{\partial\phi^2}$$

In the separable representation, $\Psi_{nlm}$ may be expressed as a product of two independent functions in the form

$$\Psi_{nlm}= R_{nl}(r)\Upsilon_{lm}(\theta,\phi) \tag{3}$$

FromEqs. (2) and (3) we get

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$$-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\left\{V(r)+\frac{\hbar^2}{2m}\left[\frac{l(l+1)}{r^2}\right]\right\}R=ER \qquad (4)$$

Since $L^2\Upsilon_{lm}=l(l+1)\Upsilon_{lm}$

The boundary condition at the interface satisfies

$$\frac{1}{m_1}\frac{d}{dr}\left(\frac{R}{r}\right)\Big|_{r=a^-}=\frac{1}{m_2}\frac{d}{dr}\left(\frac{R}{r}\right)\Big|_{r=a^+}, \qquad R(a^-)=R(a^+) \qquad (5)$$

V(r) is a step potential satisfying the heavy side function

$$V(r)=\begin{cases}=0 \ for\ r\le a\\ \\ =+\ V_o\ \ for\ r\ge a\end{cases} \qquad (6)$$

$$m=\begin{Bmatrix}m_1 & for\ r\le a\\ m_2 & for\ r\ge a\end{Bmatrix} \qquad (7)$$

The effective potential$V_{eff}$ is the same as V(r) within spherical symmetry[7,9] when $l=0$, since

$$V_{eff}=V(r)+\frac{\hbar^2}{2m}\left[\frac{l(l+1)}{r^2}\right] \qquad (8)$$

The value of the azimuthal quantum number $l=0$, and n the principal quantum number takes values n=1,2,3,….
The Radial function is a legendre function of the form [8-10]

$$R_{nl}=\sqrt{\frac{4(n-l-1)!Z^3}{[(n+l)!]^3\,n^4\,a_0{}^3}}\left(\frac{2Zr}{na_0}\right)^l.e^{-\frac{2zr}{na_0}}.L_{n+l}^{2l+1}\left(\frac{2Zr}{na_0}\right) \qquad (9)$$

$$where\ a_o=(4\pi\varepsilon_o)\hbar^2/me^2=\frac{4\pi\varepsilon_o\hbar^2}{me^2}$$

$$and\ L_{n+l}^{2l+1}(r)\ is\ associated\ Laguerre\ polynomial$$

The radius r, of the bound states are given by $\left[\frac{dR_{nl}}{dr}\right]_{l=0}=0$

$$\frac{dR_{nl}}{dr}\Big|_{l=0}=0$$

$$i.e\quad \sqrt{\frac{4(n-1)!Z^3}{(n!)^3\,n^4\,a_0^3}}\left[\left(\frac{-2Z}{na_0}\right)+\frac{n}{r}\right]e^{-\frac{2zr}{na_0}}.L_n^1\left(\frac{2zr}{na_0}\right)=0 \qquad (10)$$

The value of r is obtained from Eq. (10) by equating the factors to zero

$$\left[\left(\frac{-2Z}{na_0}\right)+\frac{n}{r}\right]=0 \qquad (11)$$

$$L_n^1\left(\frac{2Zr}{na_0}\right)=0 \qquad (12)$$

$$e^{-\frac{2Zr}{na_0}}=0 \qquad (13)$$

Consider a one electron (Z=1)dot system of GaAswith effective mass 0.067(amu),
From Eq. (11)

$$\frac{n}{r} = \frac{2}{na_0}$$

$$n^2 = \frac{2r}{a_0}$$

$$\therefore r = \frac{a_0}{2} n^2 \tag{14}$$

$$From\, Eq\, (13)$$

$$e^{-\frac{2Zr}{na_0}} = 0$$

Put $x = \dfrac{2Zr}{na_0}$ and assume harmonic approximation

$$1 - x + 2x^2 = 0$$

$$1 - \frac{2Zr}{na_0} + \frac{8Z^2 r^2}{n^2\, a_0^2} = 0$$

$$2x^2 - x + 1 = 0$$

$$x = \frac{1 \pm \sqrt{1-8}}{4}$$

$$x = \frac{1 \pm i\sqrt{7}}{4} \tag{15}$$

From Eq. (12), making r the subject, we have

$$\left[\sum_{n=0}^{n-1} (-1)^{n+1} \frac{(n!)^2\, n!}{(1+n)!.n!}\right]\left(\frac{2r}{na_0}\right)^n = 0$$

$$\left[\sum_{n=0}^{n-1} (-1)^{n-1} \frac{1}{(n+1)}\right]\left(\frac{2r}{na_0}\right)^n = 0$$

$$r = 0 \tag{16}$$

There is a maximum n permitted bound state in the dot with r = a, where a is the radius of the dot[2].

$$n = \pm\left(\frac{2aZ}{a_0}\right)^{1/2} \tag{17}$$

Though the quantum effect desired is achieved if and only if, a is of the order of the de Broglie wave length of electrons.

## 3.0 A numerical example discussion and conclusion.

For the purpose of numerical illustration of the above formalism, the GaAs dot in AlGaAs matrix is considered with electron effective mass of 0.067 and 0.15(free electron mass unit) for GaAs and AlGaAs respectively.

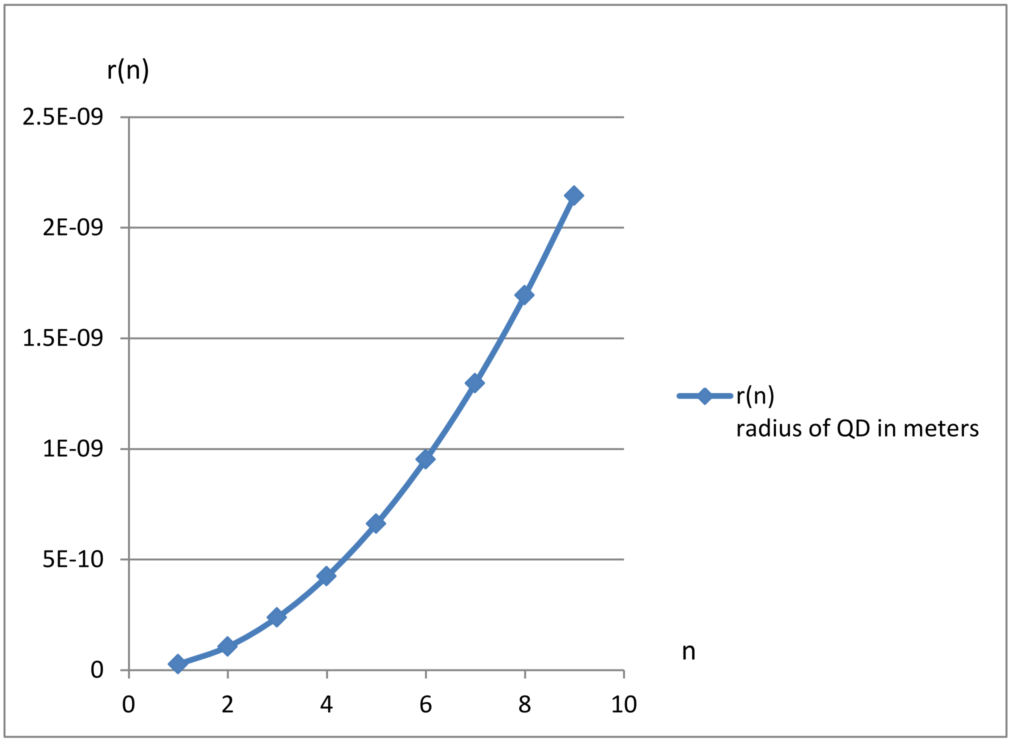


Fig 1:Real space radius r, as a function of n, the principal quantum number

Eqs.(15) and (16) do not give realistic results. Eq.(14) is practically a feasible equation and it describes the $r \propto n^2$ relationship.

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