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Exact ground state solution of shallow hydrogenic impurity states of a spherical parabolic GaAs/InAs quantum dot

F S Nmmas 

Applied Physics Department, Faculty of Science, Tafila Technical University, Tafila, 66110 Jordan

E-mail: fnmmas@ttu.edu.jo

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Abstract

The ground state spin magnetic moment current, binding energy, wave function and diamagnetic susceptibility of a shallow hydrogenic impurity located at the center of a parabolic spherical quantum dot (QD) are calculated analytically as a function of the dot size, interaction strength and confinement frequency. For comparison purposes, the results are discussed in the presence and in the absence of an impurity. Also, the dependence of the spin magnetic moment current on the spherical coordinates are derived, it is found that the spin magnetic moment current exhibits a peak structure and this current has a pronounced maximum for both small dot sizes and in the absence of impurities. Our results show that the impurities' ground state binding energy enhances as the dot dimension decreases and depends strongly on the interaction strength as the dot size increases and reduces to zero in the bulk limit for large dimensions of the dot. Moreover, the harmonic interaction has a strong influence on the diamagnetic susceptibility when the dot size increases where it decreases sharply in the presence of impurities while in the absence of impurities it decreases smoothly. In addition, the intensity of the magnetic field created by the spin magnetic moment current at the center of the QD has been calculated. It is concluded that there is a critical value for characteristic parameters and the dot size for each type of semiconductor QD to give a specific function that might be important for nanotechnology manufacturing techniques.

Keywords: spherical quantum dot, spin magnetic moment current, harmonic e-e interaction, diamagnetic susceptibility, donor impurity

(Some figures may appear in colour only in the online journal)

1. Introduction

In recent years, the growing enthusiasm for the development of nanoscience and modern uses of nanotechnology has led to the synthesis of a certain type of semiconductor called quantum dots (QD) [1]. QDs may be fabricated on semiconductor chips with the help of the electric potential of two-dimensional electron gas. A QD can be a small semiconductor area where electrons are confined to a very small size (about 100 nm) that shows a discrete spectrum of energy levels; further, the confinement potential plays an important role in the QD as it resembles the nucleus in the real atoms. For this reason, QDs are called artificial atoms [2–4]. Because of its

strikingly adjustable properties, QD innovation continues to expand and seeks to deliver their benefits to an ever-growing number of innovatively associated fields, for example solar-directed cells, transistors, lamps, medical imaging and quantitative diagnostics [1, 5–7]. The decrease in the dimensionality of QDs, created by the electrons' confinement to a smaller semiconductor region, changes its behavior exceptionally and significantly affects its optical properties and electronic structure [8–11].

Impurities play a key role in semiconductor nanostructure materials. The impurity states in these low-dimensional structures are extremely necessary because they control optical, electrical and thermal properties. Because of the

above characteristics, after the unique and pioneering work of Bastard [12] a large number of theoretical and hypothetical works on electronic structures, binding energy, optical and transport properties and diamagnetic susceptibility of hydrogenic impurities trapped in QD semiconductors with different sizes, shapes and different confinement potentials have been implemented in the literature in the last few years [13–32]. The vast majority of theoretical studies indicate that the binding energy of shallow donor impurities in nanostructure systems is strongly dependent on both the type of material and the position of the impurity, while the geometry, size and shape appear to have a minor effect [33–35].

Analytical solutions for hydrogenic impurities centered in a spherical QD have been obtained [36–38], while the perturbation method [39] and variational approach [12, 40–43] have been performed for on- and off- impurities located at the center. In particular, Porras-Montenegro *et al* [41] and Zhu *et al* [43] studied the effect of confinement and dot size on the donor binding energies (for the ground and excited states) of the impurities located at the center of QD. They demonstrated that the binding energy and its maximum depend heavily on the height of the barrier. Variational method was used to study the influence of on- and off-shallow hydrogenic impurities on the binding energy of the ground state of spherical parabolic GaAs QD [44]. The results showed that the binding energy enhanced as the dot size decreases and it increases dramatically as the impurity moves near the center.

Moreover, the utilization of external probes such as hydrostatic pressure, an electric or magnetic field, can give much profitable data about the hydrogenic impurity states [45–47]. A variational approach has been applied to a spherical QD to study the effect of a uniform magnetic field on the ground-state binding energy of an on (off)-center hydrogenic impurity [45]. The authors found that for on-center impurity, the ground-state binding energy enhances as the size of the QD diminishes, while in the presence of a magnetic field, extra increment in binding energy is found for large dot sizes. In the case of the off-center impurity, the binding energy of the ground state decreases compared with the case of the impurities in the center, and increases under the magnetic field in a smooth manner. Matrix diagonalization method had been used to study the effects of both non-parabolicity of conduction band and hydrostatic pressure on the binding energy and the diamagnetic susceptibility of a hydrogenic impurity located at the center of a spherical QD [46]. It was noted that the binding energies decreases and the magnitude of the diamagnetic susceptibility increases with decreasing pressure. Also, the absolute value of the diamagnetic susceptibility decreases in the presence of conduction band non-parabolicity at a critical value of pressure. John Peter *et al* [47] studied the binding energy of on-center shallow donors in spherical GaAs/Ga_{1-x}Al_xAs QD in the presence of electric field for three types of confinement potential. They demonstrated that the ionization energy decreases when the electric field strength increases.

Both the energy spectrum of donor electron and other characteristics of the studied impurity system can be

controlled by changing the size of the QD. One of these intrinsic properties is the spin magnetic moment current of the electron associated with its own magnetic moment. This current is not related to the charge motion, and is due to the presence of a connection between current density and magnetization. Boichuk *et al* [48] and Amirkhanyan *et al* [49] calculated the spin magnetic moment current of an impurity electron in a CdS and GaAs spherical QD, respectively. They demonstrated that the presence or absence of an impurity ion in the QD basically affects the form and the behavior of spin magnetic moment current. Mita [50] derived the spin magnetic moment current as an example of hydrogen atom. It was demonstrated that for S-states the angular current disappears, and the spin magnetic moment current is present. Many studies addressed the spin and angular current [51–53] in spherical and cylindrical QD; in such systems, it is also possible to recognize the physical conditions through which the one-electron orbital current disappears and we stay only with the spin magnetic moment current. Consequently, the fundamental feature of nanostructures is the ability to control the current value associated with the spin magnetic moment of one-electron in the studied system.

The investigations of magnetic properties in low-dimensional structures can be utilized to control and adjust the electromagnetism of nanosystems [54–56]. Additionally, the latest development of spintronics [57, 58] demands potential investigations of magnetic properties of nanostructures. One of these properties is the diamagnetic susceptibility for which we can observe quantum phenomena like, quantum chaos and electronic conductivity of electron gas in these low-dimensional structures. Many theoretical studies investigated the diamagnetic susceptibility of shallow donor impurity in a QD [59–61]. The diamagnetic susceptibility for a hydrogenic donor impurity in GaAs/Al_xGa_{1-x}As quantum well, quantum well wires and QD have been investigated [27]. The authors demonstrated the effect of dimensionality on the diamagnetic susceptibility. They concluded that when the system goes to lower dimensionality the effect of non-parabolicity becomes intangible. Using variational method Jasper *et al* [62] observed a strong influence of both the QD geometry and the confinement potential shape on the diamagnetic susceptibility of a hydrogenic donor in spherical QD. The dependence of diamagnetic susceptibility on the pressure was carried out for donor impurity confined in different dimension of QD [63]. They noticed that diamagnetic susceptibility decreases with increases in pressure.

It should be noted here that most of the previous studies on a hydrogenic donor in spherical QDs were based on theoretical approximations and numerical methods using the Coulomb interaction, so this study comes to shed light on this issue in an analytical way through a potential which mimics the Coulomb interaction, this can be achieved through harmonic interaction for which the ground-state binding energy, current of spin magnetic moment, diamagnetic susceptibility and other electronic and optical properties can be written in a closed expressions form, since no part of the Hamiltonian is neglected, therefore quantum effects show up completely in

many properties. Consequently experimentalists are invited to build up this type of model to real physical nanostructures.

The paper is organized as follows. In section 2 the mathematical formalism for the system is presented and the ground-state analytical expressions for the donor states, spin magnetic moment current, binding energy and diamagnetic susceptibility are derived. Analysis and discussion of the analytical results obtained for GaAs and InAs spherical QD are summarized in section 3. In section 4, the paper ends with important conclusions and observations.

2. Model formulation

2.1. Donor states and binding energy

Within the effective mass approximation, the Hamiltonian of shallow hydrogenic impurities located at the center of a spherical QD which is confined by a parabolic potential is given by

$$\hat{H} = \frac{\hat{p}^2}{2m^*} + \frac{1}{2}m^*\omega_0^2 r^2 + U_{\text{imp.}}(r), \quad (1)$$

where m^* is the effective mass of the electron, and ω_0 is the confinement strength frequency. The frequency of the confinement potential is related to the dot size R through the formula $\omega_0 = \frac{\sqrt{2\pi}\hbar}{m^*R^2}$ [64], \vec{r} is the position vector of the electron relative to the spherical QD center, \hat{p} is the linear momentum operator of the electron and $U_{\text{imp.}}(r)$ being the interaction potential of an electron with the impurity located at the center of the dot. In free space the Coulomb interaction proportional to r^{-1} . However, at larger distances in QD structures the Coulomb potential is screened in the presence of image charges in the contiguous layer. Furthermore, it is cut off and saturates at shorter separations because in the direction of growth the wave function of an electron has a limited extent [65]. Hence the electron-impurity interaction has been modeled by a parabolic potential [66], which makes the Hamiltonian exactly soluble and is given by

$$U_{\text{imp.}}(r) = 3V_0 - \frac{1}{2}m^*\Omega^2 r^2, \quad (2)$$

where Ω is the interaction strength and V_0 is a positive parameter which can be selected to fit different kinds of QD. The Schrödinger equation for the effective Hamiltonian in spherical coordinates (r, θ, φ) can be written as

$$\begin{aligned} & -\frac{\hbar^2}{2m^*} \left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \psi}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \psi}{\partial \theta} \right) \right. \\ & \left. + \frac{1}{r^2 \sin^2 \theta} \frac{\partial}{\partial \varphi} \left(\sin \theta \frac{\partial^2 \psi}{\partial \varphi^2} \right) \right] + \left(3V_0 - \frac{1}{2}m^*\Omega^2 r^2 \right) \psi \\ & + \frac{1}{2}m^*\omega_0^2 r^2 \psi = E\psi. \end{aligned} \quad (3)$$

Since the interaction potential and the confinement potential are spherically-symmetric, then the Schrödinger equation can be separated into the product $R(r)Y(\theta, \varphi)$ i.e.

$\psi(\vec{r}) = R(r)Y(\theta, \varphi)$, which is analogous to the problem in the hydrogen-like atom, $Y(\theta, \varphi)$ is a spherical harmonic function. The radial part of the Schrödinger equation $R(r)$ can be written as follows [67, 68]:

$$\left[-\frac{\hbar^2}{2m^*} \frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2m^* r^2} + 3V_0 + \frac{1}{2}m^*\nu^2 r^2 - \hbar\nu \left(n + \frac{3}{2} \right) \right] u(r) = 0, \quad (4)$$

where $\nu = \sqrt{\omega_0^2 - \Omega^2}$ is the effective frequency. Introducing $\alpha = \frac{m^*\nu}{2\hbar}$ and recalling that $u(r) = rR(r)$. Thus equation (4) represents the radial equation of a spherically-symmetric three-dimensional harmonic oscillator which can be solved analytically to give a normalized solution as [69]

$$R_{nl}(r) = \sqrt{\frac{2\alpha^2}{\pi} \frac{2^{n+2l+3} n! \alpha^l}{(2n+2l+1)!!}} r^l e^{-\alpha r^2} L_n^{(l+1/2)}(2\alpha r^2), \quad (5)$$

where $L_n^{(l+1/2)}$ is the generalized Laguerre polynomials; $n \geq 0$ and $l = 0, 1, 2, \dots, n-1$. The corresponding energy state of the system with impurity is given by [66, 67]

$$E_{nl} = 3V_0 + \hbar\nu \left(2n + l + \frac{3}{2} \right). \quad (6)$$

Thus, the ground state donor wave function can be reduced to

$$\psi_{000}(\vec{r}) = \left(\frac{2^7 \alpha^3}{\pi} \right)^{\frac{1}{4}} e^{-\alpha r^2} Y_0^0(\theta, \phi). \quad (7)$$

We define the S-state binding energy E_b of a shallow hydrogenic impurity as the difference between the ground-state energy of the system without Harmonic interaction, and the ground-state energy of the system with impurity, i.e.

$$E_b = \frac{3}{2}\hbar\omega_0 - \frac{3}{2}\hbar\nu - 3V_0. \quad (8)$$

2.2. Spin magnetic moment current

The expression for the wave function derived above enables us to obtain the impurity electron characteristics current, specifically the spin magnetic moment current, whose existence is due to the spin of the electron. We can obtain the expression for the spin magnetic moment current using the general form of the charge current density in non-relativistic quantum mechanics, including the electron spin and without any external fields, has the following form [70]:

$$\vec{j} = i\mu_B [\Psi \nabla \Psi^* - \Psi^* \nabla \Psi] + \mu_B \nabla \times (\Psi^* \sigma \Psi), \quad (9)$$

where $\mu_B = \frac{e\hbar}{2m^*}$ is the Bohr magneton and σ are the Pauli matrices. The first term is associated with the orbital motion of the electron and the second is the current of the spin magnetic moment. It is clear that this current is related to the presence of the correct current of spin magnetic moment, instead of the electron motion. Accordingly, the following

Table 1. Characteristic parameters for GaAs and InAs spherical QD.

	m^* (effective mass)	a_B (Bohr radius)	R_y (Rydberg constant)	ϵ (dielectric constant)
GaAs QD	$0.067m_e$	9.87 nm	5.83 meV	13.2
InAs QD	$0.042m_e$	18.4 nm	2.67 meV	14.6

relationship is always correct

$$\nabla \cdot \vec{j}_{\text{SMM}} = 0, \quad (10)$$

where \vec{j}_{SMM} is the spin magnetic moment current and it is solenoidal. Now, the electron wave function in the Russell–Saunders coupling approximation can be written as

$$\Psi_{\pm}(r, \sigma) = \psi(\vec{r}) \chi_{\pm}, \quad (11)$$

with χ_s the eigenspinors of the electron given by

$$\chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \chi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad (12)$$

since $\chi_{\pm}^\dagger \sigma \chi_{\pm} = \pm \vec{k}$, where \vec{k} is the unit vector in the direction of z -axis, then equation (9) simplified to

$$\vec{j}_{\text{SMM}} = \pm \mu_B \nabla \times [|\psi(\vec{r})|^2 \vec{k}], \quad (13)$$

in the spherical coordinate the spin magnetic moment current in the S-state ($l = 0, m = 0$) takes the following form

$$\begin{aligned} (\vec{j}_{\text{SMM}})_{ns\pm} = & \pm \frac{\mu_B}{4\pi} \left(2^{n+3} \frac{n!}{2n!} \right) \sqrt{\frac{2\alpha^3}{\pi}} \sin \theta \\ & \times \left\{ 4\alpha r [L_n^{(\frac{1}{2})}(2\alpha r^2)]^2 - \frac{d}{dr} [L_n^{(\frac{1}{2})}(2\alpha r^2)]^2 \right\} \\ & \times e^{-2\alpha r^2} \vec{\varphi}, \end{aligned} \quad (14)$$

where $\vec{\varphi}$ is the unit vector in the spherical coordinate which represents the direction in which the angle at the x - y plane is increased counter-clockwise from the positive x -axis and θ is the polar angle measured from the positive z -axis [71]. We can show through direct calculations that in the S-state ($l = 0, m = 0$) the orbital current vanishes, while the ground state ($n = 0$) spin magnetic moment current has the following form:

$$(\vec{j}_{\text{SMM}})_{0s+} = \frac{e\nu r}{4} \left(\frac{\nu m^*}{\pi \hbar} \right)^{3/2} \sin \theta e^{-2\alpha r^2} \vec{\varphi}. \quad (15)$$

2.3. Magnetic field strength at the center of QD

According to the formulas of electrodynamics, the magnetic field strength at the origin is equal to [72]

$$\vec{H}(0) = \int \frac{[\vec{r}, \vec{j}(\vec{r})]}{r^3} dV = - \int \frac{1}{r^3} [\vec{r}, [\vec{\mu}, \vec{\nabla} \rho(\vec{r})]] dV, \quad (16)$$

where $\rho(\vec{r}) = |\psi_{nlm}|^2$ and $\vec{\mu} = \mu_B \sigma = \pm \mu_B \vec{k}$. To calculate the integral (16), use the formula

$$[\vec{r}, [\vec{\mu}, \vec{\nabla} \rho(\vec{r})]] = \vec{\mu}(\vec{r} \cdot \vec{\nabla} \rho(\vec{r})) - \vec{\nabla} \rho(\vec{r})(\vec{\mu} \cdot \vec{r}). \quad (17)$$

Substituting (17) in (16), we obtain

$$\vec{H}(0) = \vec{\mu} \left(4\pi \rho(0) - \frac{4\pi}{3} \rho(0) \right) = \vec{\mu} \frac{8\pi}{3} \rho(0). \quad (18)$$

Then, the magnetic field intensity produced by the spin magnetic moment current at the QD center for the electron in the ground-state is given by

$$\vec{H}(0) = \pm \frac{4e}{3} \sqrt{\frac{m^* \nu^3}{\pi \hbar}} \vec{k} \quad (19)$$

2.4. Diamagnetic susceptibility

Diamagnetism is a material property that causes the creation of a magnetic field that opposes the effect of any magnetic field that affects the outside and produces a force of repulsion between the material and the source of the external field. Specifically, the external magnetic field changes the speed of the electron's orbit around the atomic nuclei, thereby altering the magnetic moments of the atoms. The tendency of the material to be magnetic can be measured through a diamagnetic susceptibility. For spherically symmetric charge distribution, we can assume that the x, y, z coordinates distribution are equally distributed and independent. Then $\langle x^2 \rangle = \langle y^2 \rangle = \langle z^2 \rangle = \frac{1}{3} \langle r^2 \rangle$, where r is distance of the electrons from the dot center (impurity). Thus $\langle \rho^2 \rangle = \langle x^2 \rangle + \langle y^2 \rangle = \frac{2}{3} \langle r^2 \rangle$. The volume diamagnetic susceptibility in the ground state is given by [73]

$$\chi_{\text{dia}} = - \frac{e^2}{6m^* \epsilon c^2} r^2 = - \left(\frac{e}{m^* c} \right)^2 \frac{\hbar}{4e\nu}, \quad (20)$$

where c is the speed of light and ϵ is the material dielectric constant.

3. Results and discussion

The analytical results obtained for GaAs and InAs spherical QD are performed with the characteristic parameters summarized in table 1. Throughout this study the dot radii are expressed in terms of the effective Bohr radius $a_B = \epsilon \hbar^2 / m^* k_e^2 e^2$ and the donor binding energy is expressed in terms of the effective Rydberg's constant $R_y = m^* e^4 k_e^2 / 2 \epsilon^2 \hbar^2$, where ϵ is the material dielectric constant, m^* is the effective mass of the electron and k_e is the Coulomb's constant.

In figure 1 the probability density distribution of the GaAs QD is displayed as a function of the radial coordinate r for GaAs QD for different radii ($R = a_B, 1.2a_B, 1.4a_B$) at

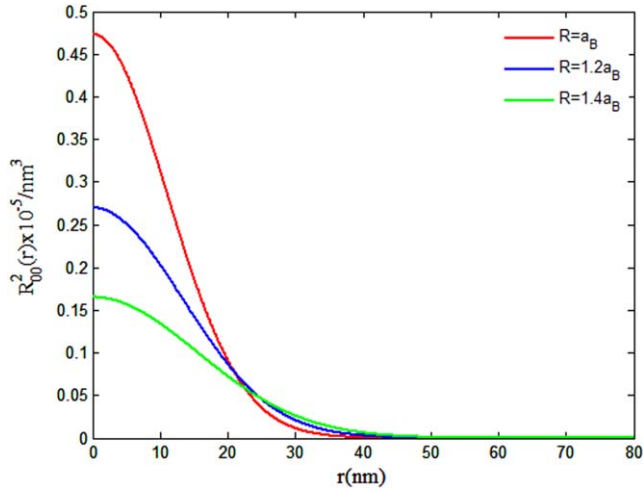


Figure 1. The probability density distribution of GaAs QD versus radial coordinate r with a shallow hydrogen-like impurity in the center for different radii at $\Omega = 1 \times 10^{12}$ Hz.

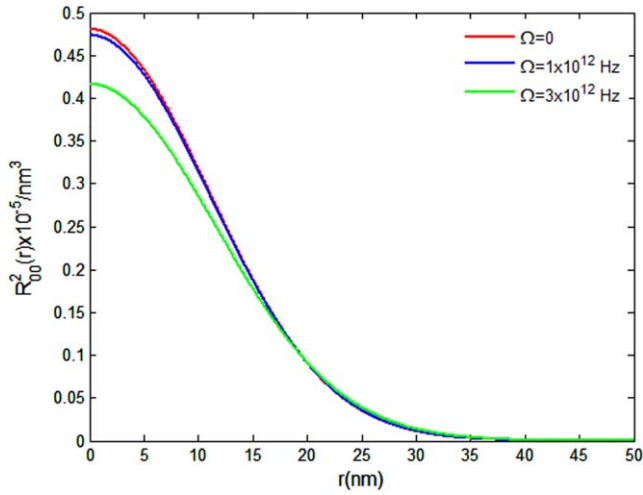


Figure 2. The probability density distribution of GaAs QD as a function of radial coordinate r with a shallow hydrogen-like impurity in the center for different interaction strength at $R = a_B$.

$\Omega = 1 \times 10^{12}$ Hz. We observe the probability densities for the donor states are maximum (strongly localized) for the on-center impurity for all radii considered and decreases as the electron moves away from the center also at large radii, i.e. $R = 1.2a_B$ and $1.4a_B$, the probability density decreases with radial coordinate less sharply than that at small radii, i.e. $R = a_B$, which is suitable because the effect of the confinement is stronger at small radii where the localization of the electron is shown noticeably. Also, it should be mentioned that as the size of the QD increases, the electron does not feel the effect of confinement and acts like an electron in the field of a hydrogen-like impurity in a bulk material. Moreover, as the size of QD increases, the curve flattens and the peak value becomes smaller.

The dependence of the probability density of GaAs QD on the radial coordinate r for $\Omega = 0, 1 \times 10^{12}$ and 3×10^{12} Hz with QD radius $R = a_B$ is shown in figure 2. The probability densities of the electron are maximum at the dot

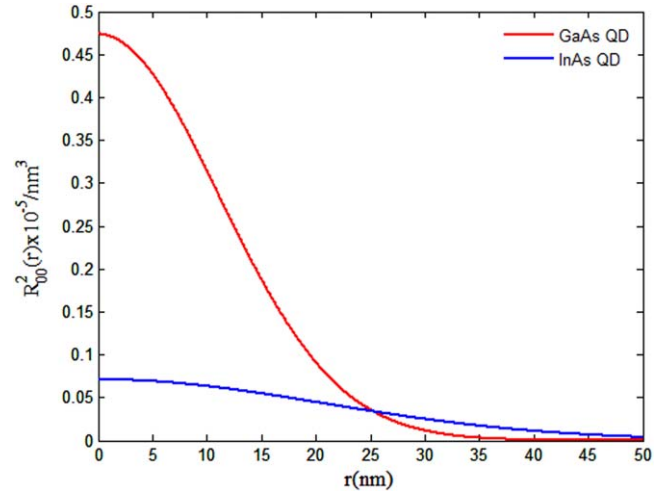


Figure 3. The probability density distribution of GaAs/InAs QD as a function of radial coordinate r with a shallow hydrogen-like impurity in the center at with $\Omega = 1 \times 10^{12}$ Hz.

center (are localized), and they were almost identical as the electron moves away from the dot center (impurity). As shown by the figure, when the electron remains close to impurity, one can notice that for strong harmonic interaction, the electron is confined weakly compared to the electron exposed to a weak harmonic interaction. Also, it is noted that the harmonic interaction decreases the probability density as r increases continuously.

In figure 3 the probability density is plotted against radial coordinate r for GaAs/InAs semiconductor QD with $\Omega = 1 \times 10^{12}$ Hz. The plot shows that the electron in GaAs QD is strongly localized more than the electron in InAs QD. The reason for this is that the Bohr radius of InAs QD is greater than that of GaAs QD. Due to this, the confinement effect appears noticeably in GaAs QD, while the donor wave function in InAs spreads all over the surrounding. As shown in the figure, the probability density is reduced with the increase in distance r , because the distance between the electron and the impurities increases, and as a result, the harmonic interaction and the quantization of size gradually become weaker.

The dependence of the spin magnetic moment current for S-state of GaAs QD on radial coordinate for a shallow hydrogen-like impurity located in the center for different radii $R = a_B^*$, $R = 1.2a_B^*$ and $R = 1.4a_B^*$ at $\Omega = 1 \times 10^{12}$ Hz and $\theta = \frac{\pi}{2}$ is shown in figure 4. The figure shows that the spin magnetic moment current peaks at a certain value of the radial coordinate ($r \sim 2a_B^*$) and then decreases at each point in space and finally it goes to zero as the electron moves away from the center of the dot (impurity); this is in conformity with the results reported by Boichuk *et al* [48]. These curves indicate that the highest peak value of the current is related to the smallest QD radius where the confinement of the impurity electron is the highest and subsequently the $R^2(r)$ dependence is rapidly varying. Also notice that as the radial coordinate increases the current gradually decreases until it completely

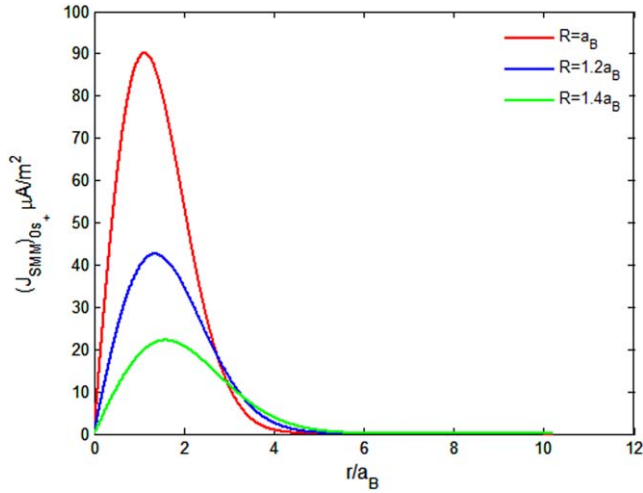


Figure 4. The spin magnetic moment current versus radial coordinate r with a shallow hydrogen-like impurity in the center of GaAs QD for different radii at $\Omega = 1 \times 10^{12}$ Hz and $\theta = \frac{\pi}{2}$.

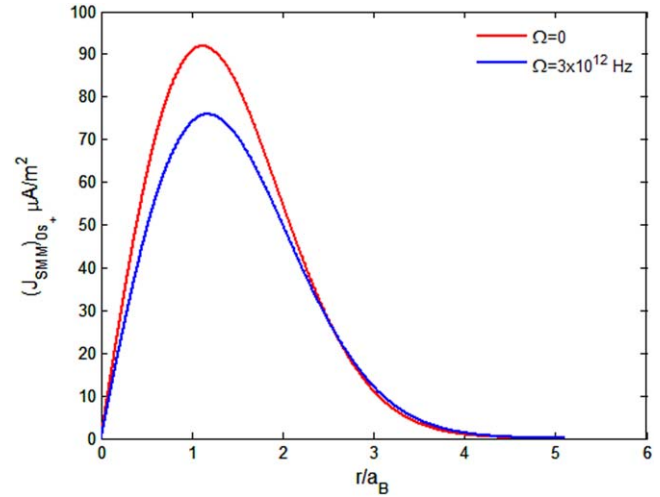


Figure 6. The dependence of the spin magnetic moment current on radial coordinate of GaAs QD in the absence and in the presence of a shallow hydrogen-like impurity at the center at $\theta = \frac{\pi}{2}$ and $R = a_B$.

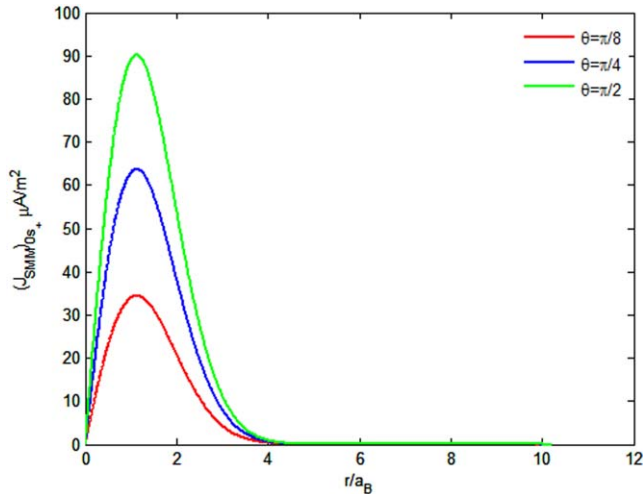


Figure 5. The spin magnetic moment current versus radial coordinate r with a shallow hydrogen-like impurity in the center of GaAs QD for different values of angle θ at $\Omega = 1 \times 10^{12}$ Hz and $R = a_B$.

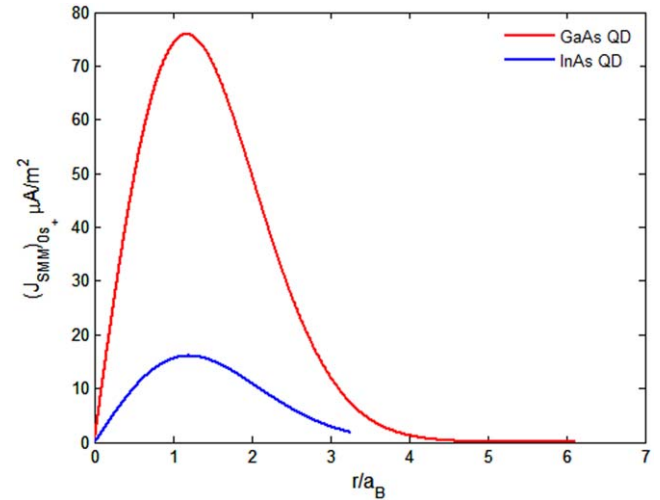


Figure 7. The dependence of the spin magnetic moment current on radial coordinate of GaAs and InAs QD at $\theta = \frac{\pi}{2}$ with $\Omega = 3 \times 10^{12}$ Hz.

vanishes; this is because the probability of localization of the electron will be zero there, see figure 1.

Figure 5 presents, for purposes of comparison, the spin magnetic moment current as a function of radial coordinate at different values of angle $\left(\theta = \frac{\pi}{8}, \frac{\pi}{4} \text{ and } \frac{\pi}{2}\right)$ for radius $R = a_B$. The figure indicates that when the electron remains close to the center of the QD (impurity), i.e. $r \sim 2a_B$, the spin magnetic moment current shows a peak structure. Moreover, the maximum value of the peak corresponds to the largest angle. Also, it is noted that decreasing the angle leads to a reduction in the current; also as the radial variable increases, the distinction of angles turns out to be less important. The major difference between figures 4 and 5 is that the peak in figure 5 shifts towards left and become narrower. The behavior of the spin magnetic moment current on radial coordinate

of GaAs QD for $\Omega = 0$ and 3×10^{12} Hz is shown in figure 6. These plots indicate that, for the same QD radius ($R = a_B$) the current peak in the absence of impurities is greater than in the case of impurities almost by one and a half times, since harmonic interaction together with confinement potential both lead to a localization of electron.

Comparison of r -dependences of the spin magnetic moments currents of an electron placed in GaAs ($a_B = 9.8$ nm) and InAs ($a_B = 18.4$ nm) QD with a shallow hydrogen-like impurity in the center is presented in figure 7. This function has a pronounced maximum for the electron distance r , which is close to the radius of QD for both semiconductors material considered. In the vicinity of $r = a_B$, we have an abrupt change in the current density, which is explained by the fact that the probability density of the electron gradually decreases, as illustrated in figure 3, as the

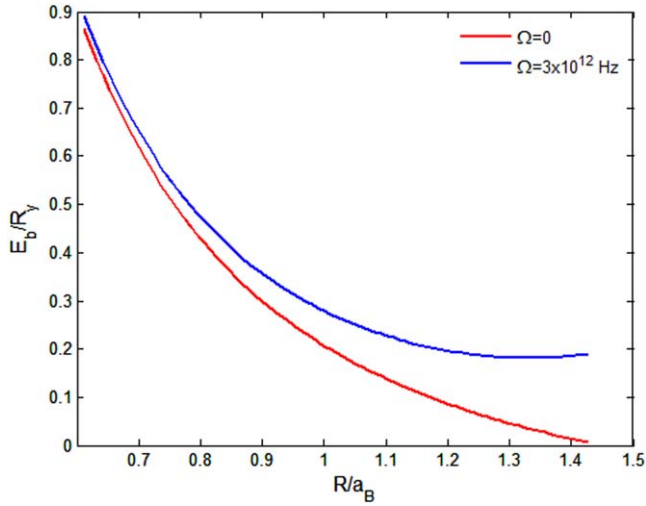


Figure 8. Variations of the ground-state binding energy with the dot size in the absence and in the presence of a shallow impurity at the center of GaAs QD for $V_0 = 0.375$ meV.

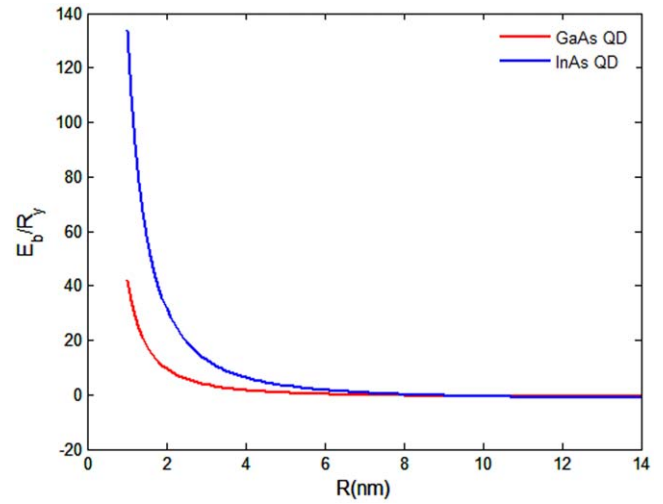


Figure 9. Variations of the ground-state binding energy with the dot size in the presence of a shallow impurity at the center of GaAs and InAs QD at $\Omega = 3 \times 10^{12}$ Hz with $V_0 = 1.875$ meV.

electron moves away from impurities, as a result the spin magnetic moment current decreases and finally it vanishes. Also, the current density produced in GaAs QD is always greater than the current generated in InAs QD. This is due to the fact that, the harmonic confinement potential is larger in the InAs QD also the energy of the electron in InAs QD near the central area is larger; see figure 9.

Figure 8 shows the dependence of the ground-state binding energy (expressed in terms of the effective Rydberg's constant) of a shallow impurity located at the center of GaAs QD on the dot size. The figure shows that the ground-state binding energy (GSBE) has a maximum value for an on-center impurity, because the electronic density has zero-order which is proportional to the wave function exhibits a maximum at the center of the QD. Also, for small radii the interaction effect has a negligible influence on the GSBE due to the dominance of the confinement energy while for large dot sizes the GSBE decreases smoothly. Actually, keeping the electron away from the center of the QD leads to a spread of a wave function gradually which basically causes a drop in the binding energy. In fact the increase in GSBE with the decrease of QD size is a common characteristic [74]. For $\Omega = 3 \times 10^{12}$ Hz one can observe that as the dot radius increases, GS binding energy increases slightly. The increase in binding energy when the radius becomes big enough is a purely quantum mechanical effect. As the QD radius becomes very large, the uncertainty in position also becomes very large and due to this the uncertainty in the momentum and hence the kinetic energy itself becomes very small and as a result binding energy increases slightly. Moreover, for sufficiently large dot radius, it is expected that the impurity behaves like a free hydrogen atom. However, our calculations show that for sufficiently large dot radius, our calculated GS binding energy is approximately $0.22 R_y$. It can be noted that, the existence of impurity at the center of QD decreases the GSBE smoothly as the dot size increases and never comes to zero and the wave

function behaves as a hydrogen atom state in free space, while in the absence of impurity the GSBE decreases monotonically until it vanishes in the bulk limit for large QD radii, since the size quantization effect becomes weaker, this is in agreement with [44] in the case of a shallow hydrogenic donor in spherical parabolic GaAs QDs using variational approach. Also, the rate of decrease in the GSBE in the absence of impurities is greater than its presence. Moreover, the existence of impurity increases GSBE for a given dot size.

The variation of the ground-state binding energy with dot size is shown in figure 9 for two QD semiconductors, i.e. GaAs and InAs QD at $\Omega = 3 \times 10^{12}$ Hz. It is noticeable that as the dot size decreases, the binding energy increases monotonically and below a certain critical value of the dot size this increase becomes very rapid, because the quantization effect becomes weaker and the interaction between the electron and the impurities increases. Also, it is clear that when the dot size increases the binding energies gradually converge and diminishes and finally it vanishes in the bulk limit for large sizes of QD. It was demonstrated that for relatively small dot size the variation in the binding energy is more pronounced for InAs QD than GaAs QD, where the InAs QD gives a higher binding energy as compared to a GaAs QD. The reason for this is that the electron wave function in InAs QD spreads more significantly to the surrounding than in GaAs QD since the surrounding is overwhelmingly controlled by hydrogenic impurity potential and not by the size of the QD. Our results are in good agreement with those reported in [41, 44].

In figure 10 we have shown the dependence of the diamagnetic susceptibility of S-state as a function of the dot radius for GaAs QD. Here we observed a decrease in the diamagnetic susceptibility when the dot size increases; this behavior is consistent with the results obtained previously in [46, 62]. The figure also indicates that, when the dot radius increases, harmonic interaction decreases the absolute value

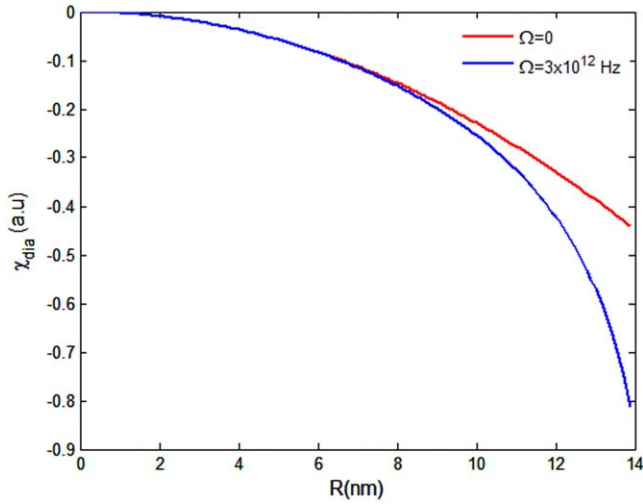


Figure 10. Ground-state diamagnetic susceptibility as a function the dot radius for GaAs QD with and without hydrogenic impurity.

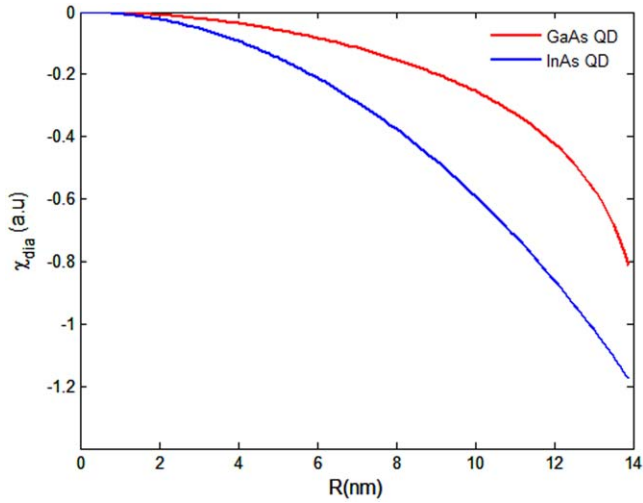


Figure 11. Comparison of the diamagnetic susceptibility with dot sizes for GaAs QD and InAs QD at $\Omega = 3 \times 10^{12}$ Hz.

of the diamagnetic susceptibility compared to the case when the impurities are absent ($\Omega = 0$). The incorporation of the harmonic interaction reduces the permeation of the wave function into the barrier of semiconductor; this in turn reduces the extended area of the wave function and actually reduces the value of $\langle r^2 \rangle$. Therefore, in accordance with equation (20), the absolute value of the diamagnetic susceptibility is reduced as the influence of the harmonic interaction. In addition, the effect of the harmonic interaction is negligible for small dot radii due to the dominance of the confinement effect. In figure 11, we compare the diamagnetic susceptibility for a hydrogenic donor in GaAs and InAs and the results are presented for $\Omega = 3 \times 10^{12}$ Hz. We observed that the susceptibility value is higher for the donor confined in GaAs spherical QD than for a donor confined in InAs spherical QD, since the wave function is highly localized and thus the magnitude of $\langle r^2 \rangle$ is higher in the GaAs QD, see figure 3. This indicates a strong influence of the QD type used in the

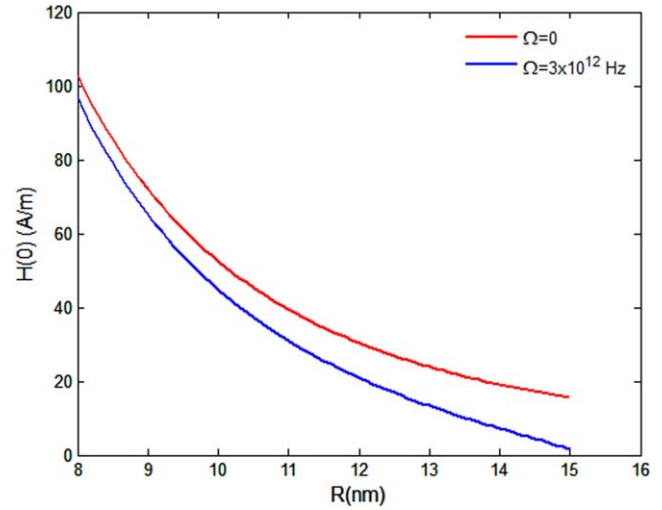


Figure 12. Dependence of the magnetic field at the center of the GaAs QD on its radius for electron in the ground-state with and without hydrogenic impurity.

semiconductors on the susceptibility. We note that the diamagnetic susceptibility of InAs QD is more sensitive to the variation of the radius for large QD than GaAs QD and converges to the limiting value of the bulk material, i.e. -1.1 a.u. The value of our diamagnetic susceptibility is justified by considering the value of the bulk limit as dot size $\rightarrow \infty$, i.e. $\langle r^2 \rangle \rightarrow 3a_B^2$ (a_B , effective Bohr radius) then $\chi_{\text{dia}} \rightarrow -1.1$ a.u. ($= -2.36 \times 10^{-6} \text{ cm}^3 \text{ mole}^{-1}$). Here we must point out that our results are in good agreement with the results presented in [27, 62].

The functional dependence of the current density from the coordinates r and θ determine the value magnetic field strength at the center of QD. From figure 12 it can be seen that the intensity decreases with the increase in the size of QD. This dependence is fully consistent with the results of the dependence of the current density on the coordinates in figure 6. For small QD size the magnetic field intensity produced in the absence of an impurity ion is higher than the magnetic field intensity produced in its presence. Also, for larger QD size the magnetic field intensity vanishes in the presence of impurity, whereas for sufficiently large size of QD this intensity comes to zero in the absence of impurity (though not shown in the figure). It is worth noting that for small QD radius the magnetic field strength created by the electron is not small. Calculations for the parameters considered in this study show that for the electronic donor it varies within $96.515 \text{ A m}^{-1} \leq H(0) \leq 102.529 \text{ A m}^{-1}$. Figure 13 shows a comparison of the magnetic field intensity produced at the center of QD for GaAs QD and InAs QD at $\Omega = 3 \times 10^{12}$ Hz. As expected, for small QD radii the magnetic field intensity decreases monotonically as the dot radius increases, also the magnetic field intensity produced in InAs QD is always higher than the intensity of the magnetic field in GaAs QD; this behavior is in consistent with the plots obtained in figure 7.

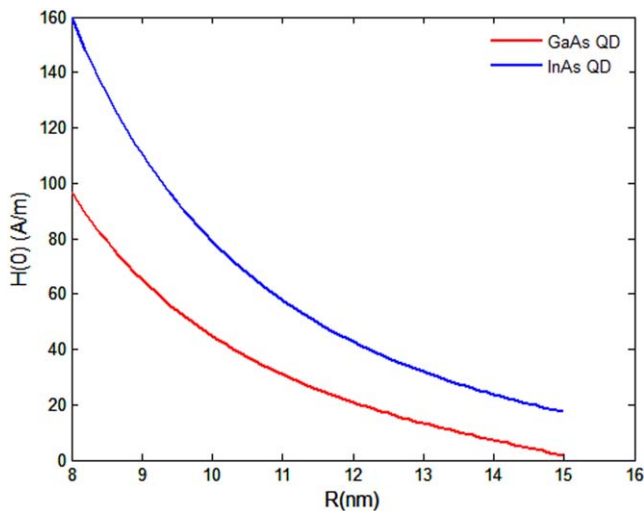


Figure 13. Dependence of the magnetic field at the center of the QD on its radius for GaAs QD and InAs QD at $\Omega = 3 \times 10^{12}$ Hz.

4. Conclusions

In this paper, within the effective mass approximation, we studied the dependence of the spin magnetic moment current, binding energy, wave function and diamagnetic susceptibility on the radial coordinate, dot size, interaction strength and confinement frequency for the electron in the ground state (S-state) coupled with shallow donor located at the center of GaAs/InAs spherical parabolic QDs. We derived the equations analytically as a function of spherical coordinates r and θ and some relevant parameters both with and without an impurity, and we compared the obtained results for both GaAs and InAs spherical QDs. It was found that the probability density for the donor states is maximum (more localized) at the origin and decreases as the electron moves away from the center. Moreover, for relatively strong interactions the localization decreases as a result to the spread of the donor wave function in all over the surrounding. Also, it was noted that the donor localization appears noticeably in GaAs QD more than InAs QD. The variation of the spin magnetic moment current with radial coordinate shows a peak structure for different sizes of the QD. It was shown that the presence or absence of an impurity in the QD as well as the size of QD essentially influence the maximum value of the spin magnetic moment current for a fixed θ . The study also proved that in the presence of impurities, the spin magnetic moment current produced by GaAs QD is always greater than that in InAs QD and the current shows a peak structure in both cases around one effective Bohr radius (for both GaAs QD and InAs QD). It was established that the harmonic interaction of an electron with an impurity reduces the spin magnetic moment current and this effect becomes tangible around $r = a_B$. It was found that the ground state binding energy decreases as the dot size increases and reduces to zero in the bulk limit when the impurity is absent. We also observed that the harmonic interaction of electron with an impurity shifts the donor levels toward higher energy levels and the effect of interaction becomes significant as the dot size increases. We compared

and showed the distinctions in behavior of an impurity ground state binding energy in GaAs and InAs spherical QDs. It was concluded that the variation in binding energy has been shown to be more pronounced and larger in InAs QD compared to GaAs QD for small QD radius. We also found that by increasing the size of the dot, the diamagnetic susceptibility diminishes rapidly with the presence of an impurity due to the harmonic interaction while it decreases slowly in the absence of impurities. It is also evident that the diamagnetic susceptibility of the donor confined in the GaAs spherical QD is higher than the donor confined in InAs spherical QD. The magnetic field intensity created by an electron at the center of the QD was derived. We have shown that the intensity of the magnetic field decreases gradually as the size of the QD increases; also the interaction of the electron with the impurities reduces the magnetic field intensity compared to the case in which the impurities are absent. It was demonstrated that the magnetic field intensity generated by InAs QD was always greater than that generated by GaAs QD, and with further increase in the QD radius, the magnetic field intensity vanishes as it expected. It is worth to mention that the electron associated with the impurity placed at the center of the quantum QD may not be affected by the environment of the QD when its radius is too large and behave just like the atom of impurity in the three-dimensional state. It was noted during this study that there are many [76] results that are consistent with previous studies, which were referred to in their appropriate positions.

We expect that the analysis conducted during this study on the donor susceptibility of a QD will be appropriate to understand the transition of metallic semiconductors [75] in low-dimensional semiconductor systems. The developing field of spintronics demands a broad investigation of magnetic properties of nano structures and furthermore encourages a comprehension of quantum chaos and electron gas conductivity in the nano systems. More investigations are required for other type of interaction potentials and for narrow QD to test the theory of effective mass approximation. We also encourage experimental efforts to support our results and the possibility of further shedding light on the donor wave function of the confined systems will soon be available. In the future, we intend to study the effect of both temperature and pressures on a hydrogenic impurity located on (off) a spherical QD center in the presence of harmonic interaction and explore other properties of these systems.

ORCID iDs

F S Nammias  <https://orcid.org/0000-0002-4245-5404>

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