Indian Journal of Pure & Applied Physics
Vol. 53, September 2015, pp. 604-611

Relativistic fine structure and the energy levels of confined multi-electron GaAs quantum dot with hydrogenic impurity within the effective mass approximation in presence of magnetic field

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Received 18 February 2014; revised 14 September 2014; accepted 11 June 2015

The theory of ground state and excited state energies calculations of multielectron quantum dot with hydrogenic impurity within the effective mass approximation has been given. Results show that ground and excited state energies decrease with dot radius. In the present paper, calculation has been carried out for two electron quantum dot. The effect of magnetic field on first excited state for different values of m_{l_1} and m_{l_2} has been studied. In addition, the first order relativistic terms such as relativistic correction to the kinetic energy, Darwin and spin-orbit interaction term for first excited state have been investigated. According to the results obtained (i) Relativistic correction to kinetic energy, Darwin and spin-orbit interaction term approaches zero when dot size increases. (ii) The splitting between j=1/2 and j=3/2 due to spin-orbit interaction decreases by increasing dot size. (iii)The splitting between j=1/2 and j=3/2 due to spin-orbit interaction decreases by increasing depth of potential.

Keywords: Quantum dot, Relativistic correction, Spin-orbit interaction, Darwin term

1 Introduction

In recent years, because of remarkable advancement in technology, it has become possible to fabricate low-dimensional semiconductor systems at nanoscale such as quantum well[1,2], quatum wires[3] and quantum dots[4-6] where charge carriers are confined in one-two and three dimensions. Quantum dots are often referred to as artificial atoms as these show atomic properties such as discrete energy levels and shell structures[7,8]. These structures being small in size play an important role in microelectronic and optoelectronic devices. Many researchers have studied the electronic structure of quantum dots[9-18].

The problem of shallow donor impurities confined to a semiconductor structure has been studied extensively in the last few years[19-21]. Studies related to impurity states are important as they play an essential role in thermal, optical and electrical properties in semiconductor devices. Hydrogenic impurity states in GaAs quantum well were first studied by Bastard[22]. External perturbations such as temperature, electric field, hydrostatic pressure, magnetic field greatly effect impurity states. Many researchers have studied the impurity states in spherical quantum dots and quantum wells under the effect of external perturbations[23,24]. The simplest confined quantum system which we can consider other than hydrogenic impurity, is the system with two electrons and helium like system. Till now there are few theoretical studies which have considered the effects of spin-orbit coupling and relativistic corrections on impurity states in a quantum pseudo dot[24,25].

In our present study, we have carried out the energies of ground and excited states and wave functions of 2-electron quantum dot with spherical harmonic oscillator type potential and also calculated the first order relativistic effects such as mass correction, Darwin term, spin orbit interaction term and our results are in good agreement[26-30].

2 Theory

We have considered here $V(r_i)$ the confining potential for i^{th} electron and is chosen as:

$$V(r_i) = -V_0 e^{-r_i^2/2R^2} \qquad \ldots(1)$$

where V_0 denotes the depth of potential and R gives a measure of the range of potential which represents the effective confinement length or size of quantum dot. Retaining up to the quadratic term after expanding potential given in Eq. (1) for $r<<R$ yields:

$$V(r_i) = -V_0 + \gamma^2 r_i^2 \quad \ldots(2)$$

where $\gamma^2 = \left(\frac{V_0}{2R^2}\right)$

and V_o can be treated as perturbation and the unperturbed Hamiltonian H_o becomes:

$$H_o = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\nabla_{r_i}^2 + \gamma^2\sum_{i}^{N} r_i^2 \quad \ldots(3)$$

where r_i (x, y, z) is the position coordinate of the i^{th} particle, m* is the effective electron mass.

In the effective mass approximation, the non-relativistic Hamiltonian of a system of two electron moving in three dimensional quantum dot in the presence of magnetic and electric field can be written as:

$$H_T = H_0 + H'_{pot} + H'_{M_1} + H'_{M_2} \quad \ldots(4)$$

$$H'_{pot} = \sum_{i=1}^{N} -\frac{e^2}{\varepsilon r_i} - NV_o \quad \ldots(5)$$

where first two terms represent hydrogenic impurity and **ε** represents dielectric constant of impurity[1-3].

$$H'_{M_2} = -\frac{q|B||L|\cos\cos\varphi}{2mc} \quad \ldots(6)$$

This term represents the energy resulting from interaction between particle's orbital magnetic dipole moment $\mu_L = qL/2\mu c$ and magnetic field B.

$$H'_{M_1} = \sum_{i=1}^{N}\frac{q^2|B^2|r_i^2\sin^2\theta}{8mc^2} \quad \ldots(7)$$

where $< r_i^2 > \sim a_o^2$, where a_0 is bohr radius, the ratio of paramagnetic and diamagnetic terms is negligible. Hence, this term is negligible.

The corresponding Schrödinger equation given in Eq. (3) is exactly soluble with the following energy spectrum in 3 dimension.

$$E_{n_i l_i} = \sum_{i=1}^{N}\hbar\omega\left(2n_i + l_i + \frac{3}{2}\right) \quad \ldots(8)$$

where $n_i, l_i = 0, \pm1, \pm2, \ldots..$

Eigen value equation for total Hamiltonian is given by:

$$H_T\psi_T = E_T\psi_T \quad \ldots(9)$$

For the non-relativistic Hamiltonian, the eigenvalue equation is given by:

$$H_o\varphi_{nlm_l} = E_{nl}\varphi_{nlm_l} \quad \ldots(10)$$

where n, l, m_l are quantum numbers of one electron wave function φ

Projecting φ_{nlm_l} into

$$\begin{aligned}
&< \varphi_{nlm_l}|H_T|\varphi_{nlm_l} > = < \varphi_{nlm_l}|H_o|\varphi_{nlm_l} > \\
&+ < \varphi_{nlm_l}|H'_{M_2}|\varphi_{nlm_l} > + < \varphi_{nlm_l}|H'_{pot}|\varphi_{nlm_l} \\
&= E^0_{nlm_l} + < \varphi_{nlm_l}| -\frac{q\vec{B}.\vec{L}}{2mc}|\varphi_{nlm_l} > \\
&+ < \varphi_{nlm_l}|\sum_{i=1}^{N} -\frac{e^2}{\varepsilon r_i} - NV_o + \sum_{i\neq j}\frac{1}{r_{ij}}|\varphi_{nlm_l} >
\end{aligned}$$

Radial Schrödinger equation can be written as :

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2mr^2} + \left(\frac{V_o}{2R^2}\right)r^2 - E_{nl}(r)\right]u_{nl}(r) = 0$$

$$-\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} - \eta^2 r^2 + \hbar\omega\left(n + \frac{3}{2}\right)\right]u(r) = 0$$

where $u(r) = rR(r)$

$$R_{nl} = N_{nl}r^l \exp\left(-\frac{\eta r^2}{2}\right)L^{l+\frac{1}{2}}_{\frac{n-l}{2}}(\eta r^2)$$

where $L_k^{\alpha}(\eta r^2)$ is a generalized Laguerre polynomial in ηr^2 and $\eta^2 = \frac{2m^* V_o}{2R^2\hbar^2}$

The normalization constant N_{nl} is:

$$N_{nl} = [\sqrt{\frac{2^{n+l+2}\eta^{l+\frac{3}{2}}}{\sqrt{\pi}}}]\sqrt{\frac{\left[\frac{n-l}{2}\right]!\left[\frac{n+l}{2}\right]!}{(n+l+1)!}}$$

where $l = n, n-2, \ldots..l_{min}$ with $l_{min} = 1$ if n is odd and $l_{min} = 0$ if n is even:

We can evaluate two electron integrals as follows:

$$< \psi_{nlm_l} \left| \frac{1}{r_i} \right| \psi_{nlm_l} >= \int | \psi_{nlm_l}(r_i, r_j, \theta, \varphi) |^2 \frac{1}{r_i} d^3 r_i d^3 r_j \quad \text{for } i \neq j$$

$$= \frac{N_{nl}^2}{2\eta^{l+1}} \int_0^\infty e^{-x_i} x_i^l \left[L_{\frac{n-l}{2}}^{l+\frac{1}{2}}(x_i) \right]^2 dx_i \qquad \ldots(11)$$

where $x_i = \eta r_i^2$

$$< \psi_{nlm_l} \left| \sum_{i \neq j} \frac{1}{r_{ij}} \right| \psi_{nlm_l} >$$

$$= \sum_{i \neq j} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \int_0^\infty \left| R_{n_1 l_1}(r_i) \right|^2 r_i^2 dr_i \int_0^\infty \left| R_{n_2 l_2}(r_j) \right|^2 r_j^2 dr_j$$
$$\int | Y_{l_1}^{m_1}(\theta_1, \varphi_1) |^2 \, d\Omega_1 \int | Y_{l_2}^{m_2}(\theta_2, \varphi_2) |^2 \times d\Omega_2 Y_1^{*m}(\theta_1, \varphi_1) Y_1^m(\theta_1, \varphi_1) \qquad \ldots(12)$$

$$\Delta E_B = < \psi_{nlm_l} \left| \frac{eBL_{iz}}{2m^* c} \right| \psi_{nlm_l} >= B\mu_B m_{l_i} \qquad \ldots(13)$$

where ΔE_B is the shift due to magnetic field. This is called Paschen-back shift and $\mu_B = \frac{e\hbar}{2m^* c}$ is Bohr's magneton.

3 Relativistic Correction

The eigen value of Hamiltonian can be further improved by including relativistic corrections such as Mass velocity, Darwin and Spin-orbit terms.

3.1 Energy Shift due to Spin-orbit Term

This term arises due to the fact that spin of moving electron changes the energy levels. Due to spin, electron behaves like a little electromagnet and a moving magnet interacts with electric field of nucleus and energy levels get changed. Spin–orbit interaction can split up spin degeneracy associated with quantum number j even without magnetic field. To calculate the Spin-orbit term, we are taking the coupled wave function as the linear combination of the spin wave function as follows:

$$\varphi_{nlj m_j} = \sum_{m_l m_s} < lsm_l m_s \mid jm_j > \varphi_{nm_l m_s}$$

where $<lsm_1m_s|jm_j>$ are Elebsch-Gordan coefficients. So that first order energy correction ΔE_{SO} is:

$$\Delta E_{SO} = < \varphi_{nlj m_j} \left| H_{SO} \right| \varphi_{nlj m_j} >$$
$$= < \varphi_{nlj m_j} \left| \sum_{i=1}^{N} \frac{1}{2m^{*2} c^2 r_i} \frac{dV_c}{dr} \vec{L}.\vec{S} \right| \varphi_{nlj m_j} >$$

where $V_c = -\frac{e^2}{\varepsilon r}$

$$\Delta E_{SO} = \frac{e^2 \hbar^2}{4m^{*2} c^2 \varepsilon} \left\{ j(j+1) - l(l+1) - \frac{3}{4} \right\} \times < \varphi_{nlj m_j} \left| \sum_{i=1}^{N} \frac{1}{r_i^3} \right| \varphi_{nlj m_j} >$$

where $j = \begin{cases} l \pm \frac{1}{2} \text{ for } l \neq 0 \\ \frac{1}{2} \text{ for } l = 0 \end{cases}$

3.2 Energy Shift due to Mass Correction

This term is relativistic correction to classical kinetic energy as it arises from relativistic variation of mass with velocity and is given below[31]:

$$H_K = -\frac{p^4}{8m^{*3} c^2}$$

Energy due to this shift is given by:

$$\Delta E_K = < \varphi_{nlm_l m_s} \left| H_K \right| \varphi_{nlm_l m_s} = -\frac{1}{2m^* c^2} \times \left[E_{nl}^2 + \sum_{i=1}^{N} \gamma^4 < r_i^4 >_{nl} - 2\gamma^2 E_n \sum_{i=1}^{N} < r_i^2 >_{nl} + \frac{\sum_i e^4}{\varepsilon^2} < \frac{1}{r_i^2} >_{nl} - \sum_{i=1}^{N} \frac{2e^2}{\varepsilon} < r_i >_{nl} E_n + \sum_{i=1}^{N} \frac{2e^2 \gamma^2}{\varepsilon} < r_i >_{nl} \right]$$

3.3 Energy Shift due to Darwin Term

Darwin term acts only at the origin as for l≠0 wave function of impurity vanish at r=0, so we only consider l=0. This term may be thought of as arising from relativistically induced electric moment of the electron and is given by:

$$H_D = \frac{\pi \hbar^2 e^2}{2m^{*2} c^2 \varepsilon} \delta(\vec{r_i}), \quad \text{where } \delta(\vec{r_i}) \text{ is Dirac delta function}$$

Energy shift due to this term is given by:

$$\Delta E_D = \frac{\pi\hbar^2 e^2}{2m^{*2}c^2\varepsilon} < \varphi_{nlm_l} \left| \delta\left(\vec{r_i}\right) \right| \varphi_{nlm_l} >$$

$$= \begin{cases} \dfrac{\pi\hbar^2 e^2}{2m^{*2}c^2\varepsilon} & \text{for } l = 0 \\ 0 & \text{for } l \neq 0 \end{cases}$$

4 Results and Discussion

In the present paper, effective atomic units (a.u.*) are used and for GaAs, the material parameters in effective atomic units are m*=1 =1 and ε=12.9. Where energy levels of quantum dot are represented by symbols n and l which are called principal and orbital quantum numbers so that levels have been shown by E_{nl}. Without magnetic field, the energies of ground state with impurity for different values of *R* and depth of the harmonic potential are presented in Table 1. As seen from Table 1 and Fig. 1 for each energy level *n*, the energy decreases as the value of *R* increases. For higher values of *R*, energy is negative.

The negative sign denotes the case where the electron binds to the impurity. It can be seen from Table 1 that the electron binds to the impurity at higher *R*. This is because the kinetic energy value is more dominant than Coulomb potential energy and the dominant value continues until larger size of quantum dot. This behaviour is the same for first excited state which we can see from Table 2 and Fig. 2. We calculate the energy of two electron quantum dot with impurity without magnetic field as a function of depth of harmonic potential for the semiconductor quantum dot GaAs as presented in Table 1. For three different values of *R* as 10, 20 and 30 nm, the results are shown in Fig. 3. For ground state, we can see that as the depth of the potential increases the energy becomes lower because as the potential minimum becomes lower, the energies would come down and the system would accommodate a large number of bound states. This behaviour of potential remains the same for first excited state as can be seen from Fig. 4 and Table 2. Table 3 present the electron energies of the first

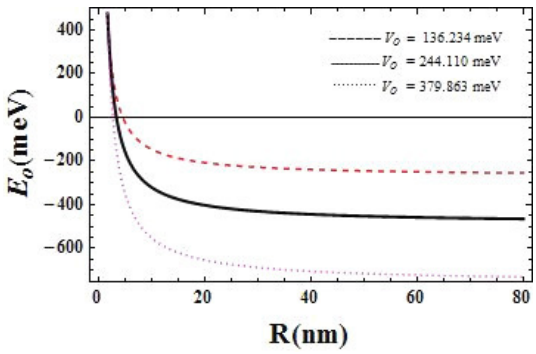

Fig. 1 — Ground state energy versus dot size for different depths of potential V_o = 136.234, 244.110, 379.863 meV

Table 1 — Ground state energy of two electron quantum dot with impurity

V=12.38367 a.u*		R=0.99a.u*	
R (in a.u*)	E_o (in meV)	V (in a.u*)	E_o (in meV)
0.099	926.882	0.0909	10.4852
0.198	332.669	0.1818	13.1089
0.297	133.753	0.2727	14.6122
0.396	33.9668	0.3636	15.5443
0.495	-26.0726	0.4545	16.1145
0.594	-66.1982	0.5454	16.4294
0.693	-94.9238	0.6363	16.5517
0.792	-116.513	0.7272	16.5222
0.891	-133.337	0.8181	16.3691
0.99	-146.82	0.9090	16.1128
1.98	-207.907	1.818	10.098
2.97	-228.537	2.727	0.7503
3.96	-238.956	3.636	-10.3071
4.95	-245.260	4.545	-22.4514
5.94	-249.494	5.454	-35.3648
6.93	-252.539	6.363	-48.8592
7.92	-254.837	7.272	-62.8126
8.91	-256.634	8.181	-77.1403
9.9	-258.080	9.090	-91.7808

Table 2 — First excited state energy of two electron quantum dot with impurity in absence of magnetic field

V=12.38367 a.u*		R=0.99a.u*	
R (in a.u*)	E_1 (in meV)	V (in a.u*)	E_1 (in meV)
0.099	1300.1	0.0909	12.8954
0.198	515.8268	0.1818	16.5817
0.297	254.1513	0.2727	18.9319
0.396	123.217	0.3636	20.5930
0.495	44.6069	0.4545	21.8146
0.594	-7.829	0.5454	22.7247
0.693	-45.3023	0.6363	23.3989
0.792	-73.4204	0.7272	23.8865
0.891	-95.2996	0.8181	24.2218
0.99	-112.8101	0.9090	24.4296
1.98	-191.7288	1.818	22.2249
2.97	-218.1138	2.727	15.8567
3.96	-231.3369	3.636	7.338
4.95	-239.2863	4.545	-2.5534
5.94	-244.5952	5.454	-13.4189
6.93	-248.3933	6.363	-25.0221
7.92	-251.2460	7.272	-37.2089
8.91	-253.4678	8.181	-49.8726
9.9	-255.2475	9.090	-62.9353

excited state as a function of magnetic field in GaAs quantum dot with R=10 nm and V_0=1 1 meV for different values of m_{l_1} and m_{l_2}. For the states $(m_{l_1} = m_{l_2} = 1)$, $(m_{l_1} = 0, m_{l_2} = 1)$, $(m_{l_1} = 1, m_{l_2} = 0)$ the electron energies increase with increase of magnetic field due to the fact that when magnetic field increases, cyclotron radius of the electron decreases. For the state $(m_{l_1} = m_{l_2} = -1)$, $(m_{l_1} = -1, m_{l_2} = 0)$, $(m_{l_1} = 0, m_{l_2} = -1)$ the electron energies decrease with increase of magnetic field as shown in Fig. 5. The introduction of magnetic field does not remove degeneracy in l but it removes partially the degeneracy in m_{l_1} and m_{l_2} as shown in Fig. 6 and Table 4.

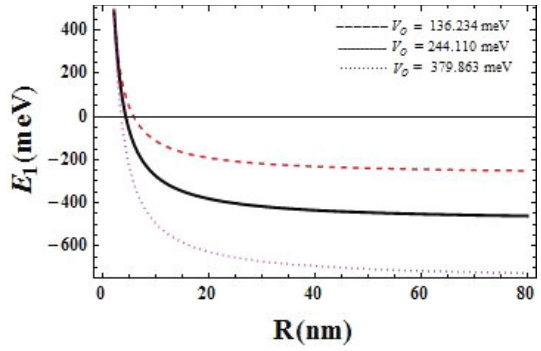

Fig. 2 — First excited state energy versus dot size for different depths of potential V_o= 136.234, 244.110, 379.863 meV

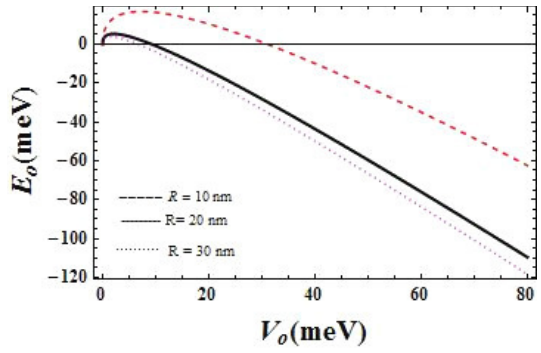

Fig. 3 — Ground state energy versus depth of potential for different dot size R= 10, 20 and 30 nm.

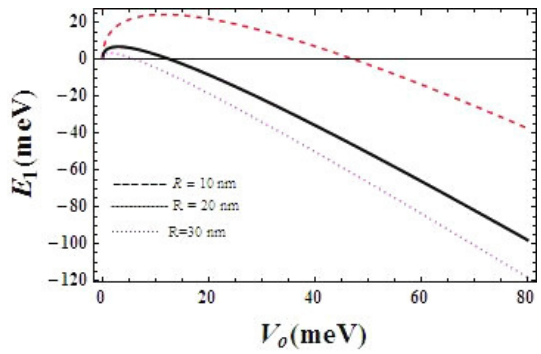

Fig. 4 — First excited state energy versus depth of potential for different dot size R= 1, 2 and 3 nm

Table 3 — Energy of first excited state with magnetic field for different values of ml_1 and ml_2 with V=0.0909 a.u.* and R=0.99 a.u.*

B(in a.u*)	ml_1=ml_2=−1 E_B (in meV)	ml_1=ml_2=1 E_B (inmeV)	ml_1=−1, ml_2=0 E_B (in meV)	ml_1=0, ml_2=1 E_B (in meV)
22.7684	6.3299	19.4610	9.6127	16.1782
45.5368	-0.2356	26.0265	6.3299	19.4610
68.3052	-6.8012	32.5920	3.0471	22.7437
91.0736	-13.3667	39.1576	-0.2356	26.0265
113.8420	-19.9322	45.7231	-3.5184	29.3093
136.6104	-26.4978	52.2886	-6.8012	32.5920
159.3788	-33.0633	58.8541	-10.0839	35.8748
182.1472	-39.6288	65.4197	-13.3667	39.1576
204.9156	-46.1944	71.9852	-16.6495	42.4403
227.684	-52.7599	78.5507	-19.9322	45.7231

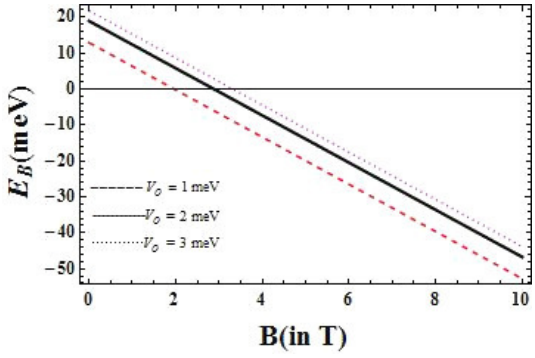

Fig. 5 — First excited state energy versus magnetic field for R=10 nm and different depth of potentials V_o=1, 2 and 3 meV

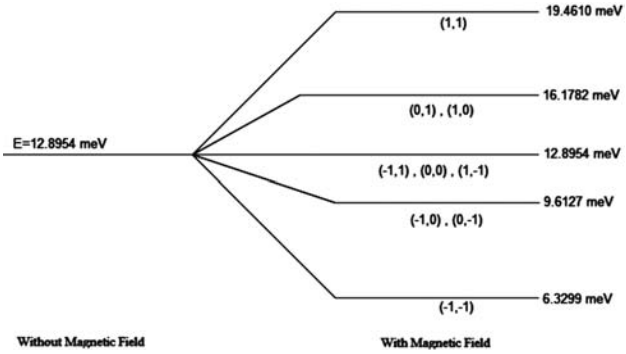

Fig. 6 — Splitting of first excited state with magnetic field for ml_1=-1 to 1 and ml_2=-1 to 1 for V=0.0909 a.u*, R=0.99 a.u.*, B=22.7684 a.u.*

The electron energies are shown for $m_{l_1} = -1$ to 1, $m_{l_2} = -1$ to 1 with V_o=1 meV, B=1T and R=10 nm. Further splitting of levels can be obtained by considering the effect of electron spins. As can be seen from Table 5, the magnitude of energy correction ΔE_K for first excited state for different values of '*R*'. The magnitude of energy correction ΔE_k increases as *R* increases. Figure 7 shows first excited state relativistic mass correction energy as a function of *R* for 3 different values of depth of potential as 136.220, 205.214 and 249.908 meV. It is also seen that relativistic mass correction energy goes to zero as *R* increases. This is because relativistic mass correction energy depends upon expectation value of 1/r and $1/r^2$. From Fig. 7, it is seen that the relativistic mass correction energy increases when depth of potential increases.

When the depth of potential increases, the wave function becomes more localized and the expectation value increases. From Table 5 and Fig. 8, we see that the magnitude of ΔE_K decreases as depth of potential increases.

The results of first order energy correction ΔE_{SO} are presented in Table 6. Spin-orbit interaction energy is plotted as a function of *R* for three different values of

Table 4 — Energy of first excited state with magnetic field for ml_1=−1 to 1 and ml_2=-1 to 1 for V=0.0909 a.u.*, R=0.99 a.u.*, B=22.7684 a.u.*

ml_1	ml_2	E (in meV)
-1	-1	6.3299
-1	0	9.6127
-1	1	12.8954
0	-1	9.6127
0	0	12.8954
0	1	16.1782
1	-1	12.8954
1	0	16.1782
1	1	19.4610

Table 5 — Mass correction energy for first excited state

V=12.38367 a.u*		R=0.99 a.u*	
R (in a.u*)	ΔE_K (in meV)	V (in a.u*)	ΔE_K (in meV)
0.099	-134.7847	0.0909	-0.0099
0.198	-33.6962	0.1818	-0.0198
0.297	-14.9761	0.2727	-0.0297
0.396	-8.4240	0.3636	-0.0396
0.495	-5.3914	0.4545	-0.0495
0.594	-3.7440	0.5454	-0.0594
0.693	-2.7507	0.6363	-0.0693
0.792	-2.1060	0.7272	-0.0791
0.891	-1.664	0.8181	-0.0890
0.99	-1.3478	0.9090	-0.0989

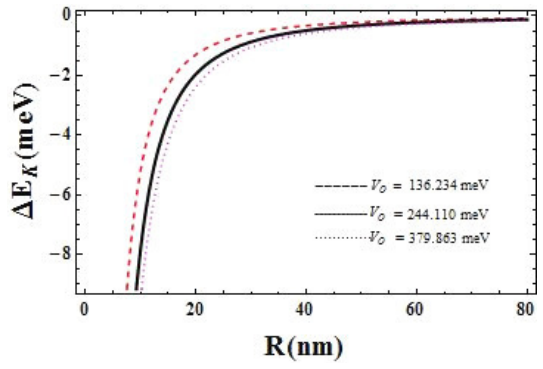

Fig. 7 — Relativistic mass correction energy versus dot size for different depth of potentials V_o= 136.234, 244.110, 379.863 meV

Table 6 — Spin orbit interaction energy for first excited state

V=12.38367 a.u.*			R=0.99 a.u.*		
j	R (in a.u.*)	ΔE_{SO} (in meV)	j	V (in a.u.*)	ΔE_{SO} (in meV)
1/2	0.099	-0.4899	1/2	0.0909	-3.8849×10^{-4}
3/2		0.2449	3/2		1.9424×10^{-4}
1/2	0.198	-0.1732	1/2	0.1818	-6.5336×10^{-4}
3/2		0.0866	3/2		3.2668×10^{-4}
1/2	0.297	-0.0943	1/2	0.2727	-8.8557×10^{-4}
3/2		0.0471	3/2		4.4278×10^{-4}
1/2	0.396	-0.0612	1/2	0.3636	-0.0011
3/2		0.0306	3/2		5.4941×10^{-4}
1/2	0.495	-0.0438	1/2	0.4545	-0.0013
3/2		0.0219	3/2		6.495×10^{-4}
1/2	0.594	-0.0333	1/2	0.5454	-0.0015
3/2		0.0167	3/2		7.4467×10^{-4}
1/2	0.693	-0.0265	1/2	0.6363	-0.0017
3/2		0.0132	3/2		8.3594×10^{-4}
1/2	0.792	-0.0217	1/2	0.7272	-0.0018
3/2		0.0108	3/2		9.2399×10^{-4}
1/2	0.891	-0.0181	1/2	0.8181	-0.002
3/2		0.0091	3/2		0.001
1/2	0.99	-0.0155	1/2	0.9090	-0.0022
3/2		0.0077	3/2		0.0011

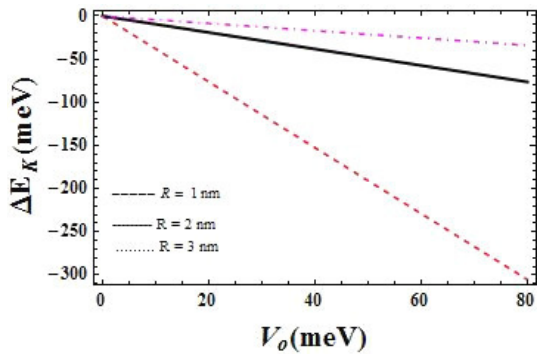

Fig. 8 — Relativistic mass correction energy versus depth of potentials for different dot size *R*=1, 2, 3 nm

depth potential as 136.220, 205.214, 249.908 meV with j=1/2 and j=3/2 in Fig. 9. The contributions coming from energy correction are positive and negative as can be seen from Fig. 9, when *R* increases, the magnitude of energy correction ΔE_{SO} decreases for j=3/2 and increases for j=1/2 and then the energies reach to a constant value. It is to be noted that spin-orbit interaction depends on total angular momentum j and expectation value of $1/r^3$. If the value of j is smaller than 1 then ΔE_{SO} is negative and ΔE_{SO} is positive for opposite case. Figure 9 shows that the level splitting decreases by increasing the depth of potential. Because due to spin of electron, it acts like little electromagnet. A moving magnet interacts with electric field of nucleus and changes the energy levels. When depth of potential increases, moving magnet becomes more confined and energy splitting decreases. Spin Orbit Interaction energy approaches to zero when *R* increases. When *R* increases, electron wave function is more spread and expectation value of 1/r is decreased. We can see from Fig. 9, level splitting is strongly dependent on *R*.

Figure 10 shows that ΔE_{SO} decreases with increasing depth of potential for j=1/2 and ΔE_{SO} increases with increasing depth of potential for j=3/2.

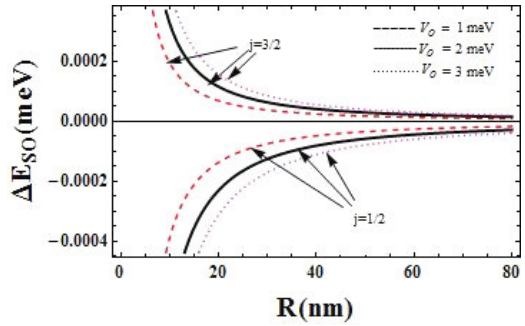

Fig. 9 — Spin-orbit interaction energy versus dot size for different depth of potentials V_o= 1, 2, 3 meV

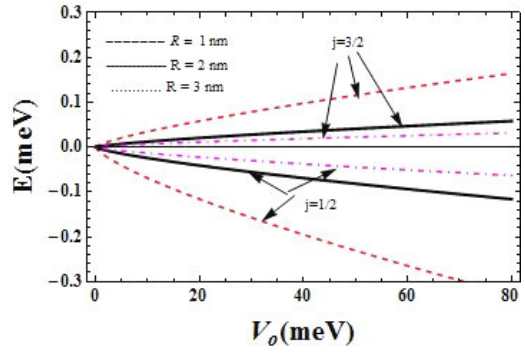

Fig. 10 — Spin-orbit interaction energy versus depth of potentials for different dot size *R*=1, 2, 3 nm

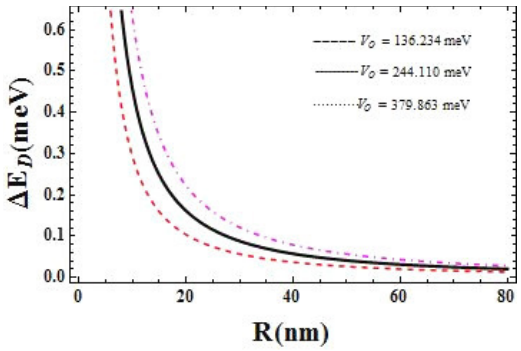

Fig. 11 — Darwin energy versus dot size for different depth of potentials V_o= 136.234, 244.110, 379.863 meV

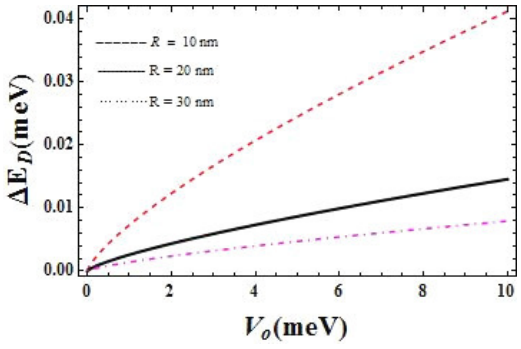

Fig. 12 — Darwin energy versus depth of potentials for different dot size *R*=10, 20, 30 nm

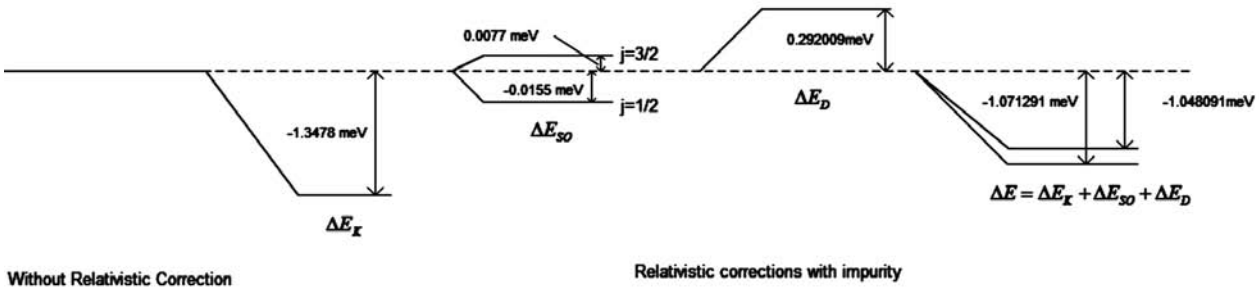

Fig. 13 — Relativistic correction energy with impurity ΔE for for first excited state for *R*=0.99 a.u*, V=12.38367 a.u*

Table 7 — Darwin energy for first excited state

V=12.38367 a.u*		R=0.99 a.u*	
R (in a.u.*)	ΔE_D (in meV)	V (in a.u.*)	ΔE_D (in meV)
0.099	9.23413	0.0909	0.0073228
0.198	3.26476	0.1818	0.0123156
0.297	1.77711	0.2727	0.0166926
0.396	1.15427	0.3636	0.0207122
0.495	0.825926	0.4545	0.0244855
0.594	0.628303	0.5454	0.0280734
0.693	0.498596	0.6363	0.031541
0.792	0.408095	0.7272	0.0348337
0.891	0.342005	0.8181	0.0380508
0.99	0.292009	0.9090	0.0411796

Level splitting decreases with increasing dot radius *R*. The result ΔE_D increases for first excited state.

As *R* increases, ΔE_D goes to a constant value. For smaller value of *R* as we increase depth of potential, the value of ΔE_D increases but as *R* increases then all curves approach to a common constant value shown in Fig. 11. Figure 12 shows that ΔE_D versus V_o for different values of *R*. As depth of potential increases, ΔE_D increases.

Figure 13 shows the total relativistic correction energy with impurity ΔE for first excited state for *R*=0.99 a.u.*, *V*=12.38367 a.u.* as shows in Table 7. We can see that ΔE is negative for both j=1/2 and j=3/2. But ΔE is more negative for j=1/2.

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