DIPOLE AND QUADRUPOLE MOMENTS OF ELECTRON IN SPHERICAL NANOLAYER

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Abstract. In this paper for one electron states dipole and quadrupole moments are studied in spherical impenetrable quantum nanolayer. It is shown that dipole moment is zero for the considered system. An analytical formula for quadrupole moment is derived. Quadrupole moment dependence upon one radius of the nanolayer, when the other one is fixed, is obtained.

1. Introduction
The development of precise methods of the growth of semiconductor nanostructures makes possible the realization of the zero-dimensional systems of different geometrical forms and sizes [1]. As we know quantum dots (QD) are those structures where quantum effects visualize themselves more vividly. Indeed, due to full quantization of the spectrum of charge carriers, QDs have similar properties to real atoms, hence, usually, QDs are called "artificial atoms" [2]. They are considered as very perspective systems, that can be used as a base elements for contemporary nanoelectronics: started from lasers based on QDs and finished with solar cells of new generation [3]-[7]. The physical processes in QDs are being investigated intensively by the specialists, as besides of pure academic interest, the results of investigation can be applicable [8]. Currently spherical, cylindrical, ellipsoidal, pyramidal, lens-shaped and many other QDs are experimentally realized and thoroughly investigated (e. g. [9] - [15]) All of these QDs listed above have specific geometries that impose their electronic, optical, kinetic and other characteristics. The latest circumstance gives a vast choice of properties of QDs for solving a concrete practical problem.

The implementation of zero-dimensional systems strongly actualized entire classes of quantum mechanical problems, which initially were carrying only academic interest and were considered as models only. In this connection it is enough to mention the problem about size-quantized film with impenetrable walls, when the system is being approximated by quantum well with rectangular infinitely high walls [16]. QD form a family of "artificial atoms" with different symmetries due to their diversity of geometries. The simplest model can be considered the "artificial hydrogen atom" consisting of QD containing one electron. Thereby we can talk about spherical, cylindrical, ellipsoidal, pyramidal "hydrogen atoms". Analogically, when the system consists of QD containing two electrons, then it is a "artificial helium atom" [17].

In order to describe two- and multi-electron states in QD it is possible to use quantum mechanical methods of description of multi-electron atoms such us: perturbation theory for helium atom and Hartree-Fock method (see for example [17] - [22]). Particularly, as it was...
shown in Ref. [23] for spherical QD it is possible to construct the analog of the Hund rule for occupation of electron shells. The authors have discussed the case when there are forty electrons in the QD. Also for that system the quadrupole moment have been computed. On the other hand, along with multi-electron systems a QD containing one electron can have dipole and quadrupole moments too. It is explained by the fact that the angular distribution of charge density in the QD is spherical symmetric only in limited cases. Particularly, it is well known that even in spherical symmetric QD only $S$-state of the electron is spherical symmetric. Thereby, spherical symmetric QD which contains one electron can have non-zero dipole and quadrupole moments. In this connection it is interesting, along with multi-electron systems, calculate these moments for one electron in a spherical symmetric QD. It is important to note that during last years the interest regarding to physical properties of layered QDs risen strongly, particularly for spherical and cylindrical nanolayers (see for example [24] - [27]). The localization of electron in spherical nanolayer can be controlled by changing both the inner radius and the outer radius. In other words in layered structures one gains additional levers to control the wave functions and energy spectrum of charge carriers. For this reason it becomes interesting to study dipole and quadrupole moments of electron in spherical nanolayer, as well as to derive the dependence of mentioned quantity on the values of inner and outer radii.

In current work the average values of dipole moment and tensor of quadrupole moment is obtained in layered spherical QD with impenetrable walls. The spin of electron is taken into account as well and hence the problem is discussed in $z$-representation of spin operators.

2. Theory

As far as we are intended to calculate quantum mechanical average values of dipole and quadrupole moments, we, definitely, need to discuss one electron states in spherical quantum nanolayer with the following confinement potential:

$$V_{\text{conf}}(r) = \begin{cases} 0, & R_1 \leq r \leq R_2 \\ \infty, & r < R_1, r > R_2 \end{cases}.$$  \hspace{1cm} (1)

With the consideration of electron spin we will find the solution of Schrödinger equation with the confinement potential (1) in $z$-representation by the matrices of Pauli, requiring the wave function to be the eigenfunction of the square of total angular momentum operator $\hat{J}_z \hat{J}_z$ and of its $z$-projection $\hat{J}_z = \hat{L}_z + \hat{s}_z \left( \hat{s}_z = \frac{\hbar}{2} \sigma_z \right)$. In the above mentioned representation for $\hat{J}_z$ and $\hat{J}_z^2$ we have [28]

$$\hat{J}_z = \hbar \left( \begin{array}{cc} -i \frac{\partial}{\partial \varphi} + \frac{1}{2} & 0 \\ 0 & -i \frac{\partial}{\partial \varphi} - \frac{1}{2} \end{array} \right),$$  \hspace{1cm} (2)

$$\hat{J}_z^2 = \begin{pmatrix} \hat{L}_z^2 + \frac{3}{4} \hbar^2 + \hbar \hat{L}_z & \hbar \hat{L}_+ \\ \hbar \hat{L}_- & \hat{L}_z^2 + \frac{3}{4} \hbar^2 - \hbar \hat{L}_z \end{pmatrix},$$  \hspace{1cm} (3)

where $\hat{L}_z = \hat{L}_x \pm i \hat{L}_y$. Considering the geometry of QD, it is more convenient to solve the problem in spherical coordinates. As far as the considered centrosymmetrical field does not depend on the spin, then the radial and angular parts can be separated and presented in the following form:

$$\Psi_{n, \ell}^{j=\ell+1/2} (r, \theta, \varphi) = \frac{F_{n, \ell} (r)}{\sqrt{2\ell+1}} \begin{pmatrix} \sqrt{\ell + m_j + 1/2} \cdot Y_{\ell, m_j - 1/2} (\theta, \varphi) \\ -\sqrt{\ell - m_j + 1/2} \cdot Y_{\ell, m_j + 1/2} (\theta, \varphi) \end{pmatrix},$$  \hspace{1cm} (4)

and
\[
\Psi_{n}^{j=\ell-1/2}(r, \theta, \varphi) = \frac{F_{n,\ell}(r)}{\sqrt{2\ell + 1}} \left( \frac{\sqrt{\ell - m_{j} + 1/2} \cdot Y_{\ell, m_{j}-1/2}(\theta, \varphi)}{\sqrt{\ell + m_{j} + 1/2} \cdot Y_{\ell, m_{j}+1/2}(\theta, \varphi)} \right), \tag{5}
\]
where \(Y_{\ell, m_{j} \pm 1/2}\) are spherical harmonics.

By presenting the radial function in the following form:
\[
F_{n,\ell}(r) = \frac{1}{r} \chi_{n,\ell}(r), \tag{6}
\]
for the function \(\chi_{n,\ell}(r)\) we come to the following equation:
\[
-\frac{\hbar^{2}}{2\mu} \left( \frac{d^{2}\chi_{n,\ell}}{dr^{2}} - \frac{\ell (\ell + 1)}{r^{2}} \chi_{n,\ell} \right) + V_{\text{conf}}(r) \chi_{n,\ell} = E_{n,\ell} \chi_{n,\ell}. \tag{7}
\]
The presence of impenetrable walls imposes boundary conditions as follows:
\[
\chi_{n,\ell}(R_{1}) = \chi_{n,\ell}(R_{2}) = 0. \tag{8}
\]
After some transformations, for the radial functions we obtain:
\[
F_{n,\ell}(r) = \sqrt{\frac{\pi k}{2r}} \left( C_{1} J_{\ell+1/2}(kr) + C_{2} J_{-(\ell+1/2)}(kr) \right), \tag{9}
\]
where \(J_{\ell \pm 1/2}(x)\) is the half-integer order Bessel function of the first kind, \(k = \sqrt{\frac{2\mu E_{n,\ell}}{\hbar^{2}}}.\) Energy spectrum of the electron, in its turn, will be defined by the circumstance of equality to zero of the following determinant:
\[
\text{det } J = \begin{vmatrix} J_{\ell+1/2}(kR_{1}) & J_{-(\ell+1/2)}(kR_{1}) \\ J_{\ell+1/2}(kR_{2}) & J_{-(\ell+1/2)}(kR_{2}) \end{vmatrix} = 0. \tag{10}
\]
Thus, for obtaining the final form of the wave functions corresponding to quantum numbers \(j = \ell + 1/2\) and \(j = \ell - 1/2,\) it is necessary to substitute (9) into (4) and (5).

Now, when we have obtained the wave functions of the system, let us turn to the dipole moment of electron in the layered QD. Dipole moment of electron equals to:
\[
P_{i} = e x_{i}, \tag{11}
\]
where \(e\) is electron charge and \(x_{i}\) is the corresponding coordinate in Cartesian coordinate system.

Let us calculate quantum mechanical average values of \(P_{i}:\)
\[
\langle P_{i} \rangle = \int \Psi_{n}^{j=\ell \pm 1/2} (r, \theta, \varphi) |^{2} P_{i} dV. \tag{12}
\]
The square of electron wave function module has the following form:
\[
|\Psi_{n}^{j=\ell+1/2} (r, \theta, \varphi)|^{2} = \frac{|F_{n,\ell}(r)|^{2}}{2\ell + 1} f^{j=\ell+1/2}(\theta), \tag{13}
\]
where
\[
f^{j=\ell+1/2}(\theta) = \left\{ (\ell + 1/2 + m_{j}) \left| Y_{\ell, m_{j}-1/2}\right|^{2} + (\ell + 1/2 - m_{j}) \left| Y_{\ell, m_{j}+1/2}\right|^{2} \right\}. \tag{14}
\]
\[ |\Psi_n^{\ell-1/2}(r, \theta, \varphi)|^2 = \frac{|F_n,\ell(r)|^2}{2\ell + 1} f_j^{\ell-1/2}(\theta), \]  
(15)

where

\[ f_j^{\ell-1/2}(\theta) = \left\{ (\ell + 1/2 - m_j) |Y_{\ell, m_j - 1/2}|^2 + (\ell + 1/2 + m_j) |Y_{\ell, m_j + 1/2}|^2 \right\}. \]  
(16)

In notations (14) and (16) we have considered that the angular part of square modulus of the wave function depends only on \( \theta \) variable.

It is easy to show that \(< P_x >\) and \(< P_y >\) equal to zero. Indeed, by substituting wave functions (4) and (5) into (12), and using well known expressions in spherical coordinate system for \( x, y \) we can assure that integrals by azimuthal angle \( \varphi \) equal to zero. \(< P_z >\) is zero too. In order to proof that we should consider the following expressions:

\[ Y_{\ell, m} \cos \theta = b_{\ell, m} Y_{\ell+1, m} + b_{\ell-1, m} Y_{\ell-1, m}, \quad b_{\ell, m} = \sqrt{\frac{(\ell + m + 1)(\ell - m + 1)}{(2\ell + 1)(2\ell + 3)}} \]  
(17)

\[ \int Y_{\ell, m}^* Y_{\ell', m'} d\Omega = \delta_{\ell,\ell'} \delta_{m, m'}. \]  
(18)

Hence we conclude that dipole moment is zero. Thereby, it is important to discuss quadrupole moment of electron as we have shown that dipole moment is zero. The tensor of quadrupole moment is defined by the following expression[29]:

\[ Q_{ik} = 3 x_i x_k - r^2 \delta_{ik}. \]  
(19)

It is a symmetric tensor of second rank \( Q_{ik} = Q_{ki} \) and the trace equals to zero:

\[ Sp \{ Q_{ik} \} = 0. \]  
(20)

Let us now turn to the calculation of quadrupole moment of electron in the spherical coordinate system. Based on the definition of the quantum mechanical average for \(< Q_{ik} >\), in general, the following can be written:

\[ < Q_{ik} > = \int |\Psi_n^{\pm\ell/2}(r, \theta, \varphi)|^2 Q_{ik} dV. \]  
(21)

Therefore, in order to calculate \(< Q_{ik} >\) we come to the following integral:

\[ < Q_{ik} > = \int \left\{ \frac{|F_n,\ell(r)|^2}{2\ell + 1} \int Q_{ik} f_j^{\pm\ell/2}(\theta) d\Omega \right\} dr, \]  
(22)

where \( d\Omega \) is the element of solid angle.

Based on the definition of tensor \( Q_{ik} \) (19) with direct calculations can be shown, that the average values of nondiagonal components are equal to zero:

\[ < Q_{xy} > = < Q_{yx} > = < Q_{yz} > = 0. \]  
(23)

For diagonal components in its turn can be shown that the following equations takes place: [28]

\[ < Q_{xx} > = < Q_{yy} > = -\frac{1}{2} < Q_{zz} >. \]  
(24)

Therefore, the problem reduces to calculating the integral:
The integration by angles can be achieved using the relation
\[
\mathcal{I} (3 \cos^2 \theta - 1) |Y_{\ell, m} (\theta, \varphi)|^2 (\theta) d\Omega = \frac{2 \ell (\ell + 1) - 6 m^2}{(2\ell - 1)(2\ell + 3)}.
\] (26)

After the calculations, the details of which can be found in [28], the expression (25) will be written in the following form:
\[
< Q_{zz} > = \frac{1}{2} \left( 1 - \frac{3m_j^2}{j (j + 1)} \right) I_{n, \ell} (R_1, R_2),
\] (27)
where the following notation is introduced
\[
I_{n, \ell} (R_1, R_2) = \int_{R_1}^{R_2} |F_{n, \ell} (r)|^2 r^4 dr.
\] (28)

Let us note, that the formula (27) is correct both for the value of quantum number \( j = \ell + 1/2 \) and for \( j = \ell - 1/2 \).

Finally, for our case we can write the electrostatic field of the system as follows:
\[
\varphi (r) = \frac{q}{\varepsilon r} + \frac{1}{2 \varepsilon r^5} \sum_{ik} < Q_{ik} > x_i x_k,
\] (29)
where \( i, k = x, y, z \) and \( \varepsilon \) is the average dielectric constant of surrounding medium. Here we have considered that dipole moment of this system is zero. As far as \( < Q_{ik} > \) is equal to
\[
< Q_{ik} > = \frac{1}{2} \left( 1 - \frac{3m_j^2}{j (j + 1)} \right) I_{n, \ell} (R_1, R_2) \begin{pmatrix}
-\frac{1}{2} & 0 & 0 \\
0 & -\frac{1}{2} & 0 \\
0 & 0 & 1
\end{pmatrix},
\] (30)
therefore, for electrostatic field can be written:
\[
\varphi (r) = \frac{q}{\varepsilon r} + \frac{< Q_{zz} >}{4 \varepsilon r^3} \left( 3 \cos^2 \vartheta - 1 \right) = \frac{q}{\varepsilon r} + \frac{1}{8 \varepsilon r^3} \left( 1 - \frac{3m_j^2}{j (j + 1)} \right) I_{n, \ell} (R_1, R_2) \left( 3 \cos^2 \vartheta - 1 \right),
\] (31)
where \( \vartheta \) is the angle between \( \vec{r} \) radius vector of observation point and \( OZ \) axis.

3. Discussion
Quadrupole moment of electron in spherical symmetric field, regardless of the form of its potential, possesses an important characteritics connected with the presence of the spin. By direct calculation it can be shown, that the relation \( < Q_{zz} > / I_{n, \ell} (R_1, R_2) \) equals to zero at a value \( j = 1/2 \) both for the states \( S_{1/2} \) and \( P_{1/2} \). Thus, spherical symmetry can possess not only the \( S \) state but also the \( P \) state. If we consider a similar task without spin, then we can see that a spherical symmetry occurs only for the state \( S \). On figures 1, 2, 3 and 4 it is represented the dependence of \( I_{n, \ell} (R_1, R_2) \) quantity on one radius of the nanolayer when the other one is fixed for different orbital and radial quantum numbers \( n \) and \( \ell \). From these figures, obtained by numerical calculations, we can conclude that:
1) Quadrupole moment increases for both cases when inner radius increases and outer is fixed and when outer radius increases and inner one is fixed. Moreover, from corresponding curves we can see that quadrupole moment increases more rapidly for the case when inner radius increases than for the case when outer radius increases. Hence, we can proof that spherical symmetry violation takes place for both cases but for the case when inner radius increases the spherical symmetry violation takes place more rapidly. Also we should note that for the case of spherical quantum dot (see figure 2 or 4) quadrupole moment tends to zero when outer radius $R_2$ tends to zero. This is because spherical quantum dot becomes sufficient small so that we could neglected the non-spherical distribution of electron in the space. In other words, by decreasing the radius of spherical qunatum dot we restore spherical symmetry, hence quadrupole moment becomes closer to zero.

2) When radial quantum number increases ($n$) and all other parameters are constant ($\ell, R_1, R_2$) quadrupole moment decreases. Furthermore, when we increase $n$ it goes to saturation.
We should also note that for the case of spherical QD (see figure 2) when \( R_2 \) is sufficiently small then the dependence of quadrupole moment from \( n \) weakens. Particularly, we can say there is no dependence on \( n \) for sufficiently small outer radii. Whereas, for the case of spherical nanolayer the dependence is weaker as bigger the inner radius \( R_1 \) is. Particularly, we can say there is no dependence on \( n \) for sufficiently big inner radii (see figure 1).

3) When orbital quantum number increases (\( \ell \)) and all other parameters (\( n, R_1, R_2 \)) are constant quadrupole moment increases in contrast with the radial quantum number case. Here also quadrupole moment value has a saturation when we increase \( \ell \) (see figure 3 and 4). We should also note that for the case of spherical QD (see figure 4) when \( R_2 \) is sufficiently small then the dependence of quadrupole moment from \( R \) weakens as it was for the previous case. Particularly, we can say there is no dependence on \( \ell \) for sufficiently small outer radii. Whereas, for the case of spherical nanolayer the dependence is weaker as bigger the inner radius \( R_1 \) is. Particularly, we can say there is no dependence on \( \ell \) for sufficiently big inner radii (see figure 3).

As we already noted, in case when the quantum number of orbital moment is fixed (\( \ell = 2 \)) and we discuss different values for radial quantum number \( n \) \((n = 1; 3; 6)\) with increase of \( R_1 \) the curves of \( I_{n,\ell} (R_1, R_2) =< r^2 \rangle \) come closer to each other. This is an expected result as far as \( < r^2 > \) for very small thickness of the nanolayer for \( n = 1; 3; 6 \) approximately will have same value. Therefore, quadrupole moment will be defined by angular distribution which, in its turn, is defined by the following coefficient: \( (1 - \frac{3n^2}{J(J+1)}) \) which is constant for fixed angular and spin quantum numbers. We should also note that the same situation takes place for the case when \( n \) is fixed and \( \ell = 2, 3, 4 \):

\[
< r^2 >_{n,2} = < r^2 >_{n,3} = < r^2 >_{n,4}.
\]  

This interpretation also explains the saturation effects discussed above with increase of \( n \) when \( \ell, R_1, R_2 \) are fixed and with the increase of \( \ell \) when \( n, R_1, R_2 \) are fixed. These facts are being obvious from the curves of square of modulus of radial function for different \( n \) and \( \ell \) from \( R_1 \) to \( R_2 \). Moreover, those curves demonstrate that with the increase of \( n \) saturation tends to a small values of \( I_{n,\ell} (R_1, R_2) \) while with the increase of \( \ell \) the values of \( I_{n,\ell} (R_1, R_2) \) increase and saturation takes place for bigger values.

4. Conclusion

In this paper for one electron states dipole and quadrupole moments are studied in spherical impenetrable quantum nanolayer. It is shown that dipole moment is zero for the considered system. An analytical formula for quadrupole moment is derived. Quadrupole moment dependence on one radius of the nanolayer, when the other one is fixed, is obtained for different radial (\( n \)) and orbital (\( \ell \)) quantum numbers. The dependence of quadrupole moment on orbital and radial quantum numbers when other parameters are fixed is discussed in details.

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