Nonlinear optical properties of cylindrical quantum dot with Kratzer confining potential in the presence of axial homogeneous electric field

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Abstract. Electronic states of an electron localized in a cylindrical quantum dot with Kratzer confining potential in the presence of axial electrostatic field are considered. The dependences of the dipole matrix elements on the geometrical parameters and values of the electric field are calculated. Nonlinear optical effects such as second harmonic generation and optical rectification in this structure are studied. The electric field values, at which double resonance condition are satisfied, have been found. Optical rectification and the second harmonic generation coefficients of energy dependence curves are obtained. Specificity of the Kratzer confinement potential profile leads to vanishing of the mean displacement of the electron in intraband transitions. This fact is reflected in the behavior of optical rectification coefficient, which has a deep dip around certain values of the electric field.

1. Introduction
Optical properties of quantum dots (QDs) have always attracted the researchers attention because the results of their theoretical investigation can be directly applied in nanotechnology [1, 2]. In contrast to real atomic systems, QDs are characterized by large values of dipole matrix elements [3]. Due to this fact, QDs can be considered as promising candidates for application in semiconductor optoelectronic devices of the new generation [1, 4]. Besides linear optical characteristics of QDs, their nonlinear properties cause interest of researchers because many nonlinear effects such nonlinear optical absorption, the refractive index change, optical rectification (OR), second harmonic generation (SHG), etc. can be employed to create new optoelectronic devices [5].

2. Theoretical calculations
Let us consider GaAs cylindrical QD (figure (a)) in the presence of an axially directed uniform electric field with substrate region as the lower medium $z \leq 0$, where $z$ is coordinate in the growth direction $(OZ)$ axis). Due to inter-diffusion effects in the axial direction one-dimensional Kratzer potential is considered given by the following formula (see figure 1 (b)) [6]:

$$V_{conf}(z) = \begin{cases} 
-2D \left( \frac{\alpha}{z} - \frac{\alpha^2}{2z^2} \right), & (0 < z < L) \\
\infty, & z > L, z < 0
\end{cases}$$

(1)

where $D$ - depth parameter, $\alpha$ determines width of the potential and $L$ is height of the cylinder.
Performing separation of variables for Schrödinger equation in the axial direction one can write:

\[
\left(-\frac{\partial^2}{\partial z^2} - 2D\left(\frac{\alpha}{z} + \frac{\alpha^2}{2z^2}\right) + \gamma z\right)\chi(z) = E\chi(z),
\]  

where \(\gamma = -0.17 \cdot 10^{-3} (\text{cm/V}) \cdot F (\text{V/cm})\) - dimensionless electric field strength measure for GaAs, \(F\) - electric field strength, \(\mu\) - effective mass of the electron. In present work all the lengths are measured in the effective Bohr radius \(\alpha_B = \hbar^2 e/\mu \epsilon^2\), and energy - in effective Rydberg constants \(E_B = \hbar^2/2\mu \alpha_B^2\), \(\epsilon\) is dielectric permittivity of QD.

The boundary conditions for axial equation (2) are as follows: \(\chi(0) = 0\), \(\chi(L) = 0\). The similar equation without electric field have been investigated and analytical expressions for energy spectrum and wave function have been carried out in [7]. However, the addition of the electric filed term in the axial Schrödinger equation greatly complicates finding an analytical solution, therefore we solve it by using the finite element method [8]. The region \(z \in (0, L)\) was discretized with elements with maximum element size \(10^{-4}\).

Calculating matrix elements \(\mu_{ij}\) for non-diagonal transitions \(i \neq j\), as well as the average electron displacement during the transition \(\delta_{ij}\), defined in [9, 10]:

\[
\mu_{ij} = \left< \chi(z), \chi(z) \right>, \quad i, j = 0, 1, ..., \quad i \neq j,
\]

\[
\delta_{ij} = \left< \chi(z), \chi(z) \right> - \left< \chi(z), \chi(z) \right>, \quad i, j = 0, 1, ..., \quad i \neq j.
\]

The expressions for nonlinear coefficients can be obtained using below mentioned formulas. The expression for the SHG coefficient in the case of double resonance \(\omega \approx \omega_1 \approx \omega_2\) can be obtained by solving time-dependent one-electron density matrix equation with intraband relaxation using the iterative method, expanding density operator into infinite series [11]:

\[
\chi_{\text{SHG}}(2\omega) = e^i \sigma_{\epsilon} \frac{|\mu_{12} \mu_{23} \mu_{31}|}{\epsilon_0 \hbar^2 \left(\omega - \omega_1 - i\Gamma_2\right) \left(2\omega - \omega_2 - i\Gamma_3\right)}.
\]

and using the expressions for a two-level quantum system OR coefficient [12]:

Figure 1. (a) Schematic view of the studied system; (b) truncated Kratzer potential.
\[ \chi_0^{(2)}(0) = \frac{4e^3 \sigma_s}{\varepsilon_0 \hbar^2} |\mu_{12}\delta_{12}| \frac{\omega_{12}^2 \left(1 + \frac{T_1}{T_2}\right) + \left(\omega^2 + \frac{1}{T_2^2}\right) \left(\frac{T_1}{T_2} - 1\right)}{\left(\omega_{12} - \omega\right)^2 + \frac{1}{T_2^2} \left(\omega_{12} + \omega\right)^2 + \frac{1}{T_2^2}}. \]  

(6)

Here, \( \omega_{12} \) is the transition frequency corresponding to the difference between the energies of the first excited state and the ground state, \( \sigma_s \) is the electron density in the QD, \( T_1 \) is the longitudinal relaxation time, and \( T_2 \) is the transverse relaxation time. The inverse lifetime for the first \( \Gamma_{21} \) and second \( \Gamma_{31} \) excited states will be considered equal \( \Gamma_{21} = \Gamma_{31} = \Gamma \). The position of the resonance peak of the SHG coefficient under the condition of two-photon resonance \( \chi_{\text{SHG,max}}^{(2)}(2\omega) \) is defined as:

\[ \chi_{\text{SHG,max}}^{(2)}(2\omega) = \frac{e^3 \sigma_s |\mu_{12}\mu_{23}\mu_{31}|}{\varepsilon_0 \left(\hbar \Gamma\right)^2}. \]  

(7)

3. Results and discussions

The following parameters have been used in the calculations: \( L = 4a_B \), \( \alpha = 1a_B \), \( D = 30E_B \approx 175meV \), relaxation times \( T_1 = 1ps \), \( T_2 = 0.2ps \) [13], and electron density \( \sigma_s = 10^3 cm^{-3} \). The dependence of the first three energy levels on the electric field is shown in figure 2:

![Figure 2](image1)

Figure 2. (a) The dependence of the first three energy levels on the electric field strength; (b) The dependence of \( \hbar\omega_{32} - \hbar\omega_{21} \) on the electric field value.

Figure 2 (a) shows the dependence of the first three energy levels on the electric field strength \( n = 1,2,3 \). Energy levels rise in absolute value with increasing field, however, there are such values of the electric field, at which the distance between the first and second levels is equal to the distance between the second and third levels. Fulfillment of this condition is necessary for observing the SHG. In order to determine the indicated values of the electric field, figure 2 (b) shows the dependence of the difference in energy distances between the levels \( \Delta E_{21} = \hbar\omega_{21} \) and \( \Delta E_{32} = \hbar\omega_{32} \). As follows from this figure, this difference \( \hbar\omega_{32} - \hbar\omega_{21} \) is a non-monotonic function on the electric field value. Moreover, the equidistance of the levels is realized for value \( F = 22kV/cm \) and \( F = 55kV/cm \).
Figure 3. (a), (c) SHG coefficient dependence on incident photon energy for different electric field values; (b), (d) $|\mu_{12}\mu_{23}\mu_{31}|$ dependence on electric field values.

In accordance with double resonance condition SHG dependence on the incident photon energy is shown above (see figure 3). The figure 3 (a) and (c) show the dependence of SHG coefficient on incident photon energy, where the expression $|\mu_{12}\mu_{23}\mu_{31}|$ defines the SHG peak height. The matrix elements included in the expression for the SHG coefficient (see (5)) are determined by the overlap of the wave functions of the corresponding states. The behavior of the absorption curves around the resonant points $F = 22 kV / cm$ and $F = 55 kV / cm$ are significantly different. As can be seen from figure 3 (a), the absorption peaks around the point $55 kV / cm$ for the higher values of the electric field undergoes a blue shift. This is due to the fact that the distance between the third and first energy levels $\hbar\omega_{31} = \hbar\omega_{32} + \hbar\omega_{21}$ increases with the electric field increase (see Table 1). In addition to that, the overlap integral monotonously decreases, which explains the decrease in peak values of the SHG coefficient. As can be seen in figure 3 (b), when the values of the electric field $F = 52 kV / cm$, the specified overlap is expressed most clearly in comparison with $F = 55 kV / cm$ and $F = 58 kV / cm$. The reverse picture appears around the point $22 kV / cm$ (see figure 3 (c), and figure 3 (d)). The value of the expression $|\mu_{12}\mu_{23}\mu_{31}|$ increases with the electric field increase, which indicates the strengthening of the corresponding overlap integrals. At the same time, the inter-level distance $\hbar\omega_{31}$ around a point $F = 22 kV / cm$ decreases with electric field increase, therefore in this case there will be a redshift, as it is shown in figure 3 (c).
The figure 4 (b) shows $|\mu_{12}\delta_{12}|$ curve dependence on the electric field value. This curve has a sharp dip in the area $38kV/cm$. This is associated with the dependence of $\delta_{12}$ on the electric field. As one can see from its definition, this value is the difference between the $z$ coordinate average values for the ground and first excited states. Increasing the electric field lead to an increase of the average value of $z$ coordinate for the ground state and decrease for the excited one. At some point they become equal and the $\delta_{12}$ vanishes, this is the reason for such sharp dip in the figure 4 (b). As the result this fact is reflected on the OR coefficient dependence curves. Figure 4 (a) shows the dependence of the coefficient of optical rectification of the incident photon energy. Since there is a sharp dip of around $38kV/cm$, the peak of the corresponding OR curve assumes a slight height. With a field value of $45kV/cm$ and $30kV/cm$, we have the largest value of the OR curve peak. Note that in the considered case, unlike other models of a confining potential, there is a dip in the bottom of the potential curve. This fact is reflected in the energetic, electronic, and optical properties of such structures. Thus, the vanishing of the coefficient of OR in a narrow range of values of the electric field is a consequence of this fact.

4. Conclusion
The cylindrical quantum dot with Kratzer confining potential in the presence of axial electrostatic field is considered. It has been shown that there are certain ranges of electric field value at which the double resonance condition is satisfied. The OR and the SHG coefficients curves on the energy of the incident light has been investigated. It has been demonstrated that the double resonance condition satisfied around values $22kV/cm$ and $55kV/cm$ of the electric field. The SHG coefficient peak is shifting to the higher energy region with the electric field increase around values $22kV/cm$, on the other hand, we observe redshift around values $55kV/cm$. It has been demonstrated that OR curve peaks show a non-monotonic behaviour with the electric field increase, which is associated with corresponding dipole matrix elements non-monotonic dependence on the electric field. Also it has
been shown that the dependence of OR coefficient intensity peak has a sharp dip at the electric field value $38 \text{ kV/cm}$. Note, that the specificity of the Kratzer potential lead to appearance of vanishing effect of the OR coefficient in a narrow range of values of the electric field.

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