ISSN 1512-1461

UDC 539

THE EFFECTS OF THE OPTICAL ANISOTROPY FOR THE SYSTEM WITH ONE ELECTRON CONFINED IN ELLISPOIDAL POTENTIAL WALL

Z. S. Machavariani

Department of Physics, Faculty of Exact and Natural Sciences, Ivane Javakhishvili Tbilisi State University,
Chavchavadze Avenue 3,0179 Tbilisi, Georgia
e-mail: zaal.machavariani@tsu.ge

Abstract. *The optical properties of anisotropic quantum dots of ellipsoidal shape are investigated and discussed as a function of the dot aspect ratio. The optical matrix elements in the dipole approximation are calculated. The main result is that optical processes significantly depend on the radiation polarization.*

Keywords: Quantum dot, Dipole transition, Potential wall

Introduction

The interest in quantum dots (QD) and, more generally, semiconductor nanostructures has been growing in the last two decades. The interesting feature of such structures is that as the system dimensions become smaller than the particle de Broglie wavelength, the physical properties are modified by quantum confinement. It is known, for example, that the optical gap increases on decreasing the mean dimensions, giving rise to a blue-shift of the optical spectra, and that a discrete set of states appears as an effect of reducing the system dimensionality. This has given rise to the possibility of a number of new, very interesting applications, such as producing artificial atoms and molecules [1], single-electron transistors [2] and quantum dot lasers [3].

In the theoretical works, it is customary to assume a spherical shape for the quantum dot (SQD). Since the deformation of spherical shape during quantum dot growth is unavoidable, quantum dot with an ellipsoidal shape represents a better approach to the actual problems [4]. A theoretical research of ellipsoidal quantum dots (EQD) was carried out in [4–8], where the energy spectra of a charged particle and an exciton were found, and the influence of polarization effects on the quasiparticle spectrum was studied. These calculations were performed for an infinite potential well which can be used either for a QD of a large volume or when the band gap at the interface is sufficiently large [9]. Some interesting features of anisotropic nanostructures can also be found in [10], where the quantum dot anisotropic geometry is studied within the pertubation theory as a deformation with respect to the spherical dot.

In parallel, theoretical and experimental investigations have been performed on the study of the nonlinear optical properties of QD. For instance, Xie [11] investigated the optical properties of SQD with parabolic confinement potential containing one electron and a donor (acceptor) impurity in the presence of an electric field. Xie [12] also investigated the nonlinear optical rectification (OR) of a confined exciton in a disc-like QD with an applied electric field. Guo et al. [13] studied the nonlinear OR in parabolic quantum wells with an applied electric field.

Sadeghi [14] investigated the linear and nonlinear optical absorption coefficients of an EQD containing electron in the presence of external electric filed and a donor (acceptor) impurity. The nonlinear optical properties of a hydrogenic impurity in an ellipsoidal finite potential has been analyzed by Rezaei [15]. The effect of surface polarization charges due to impurity on the impurity binding energy is considered in [16]. The results clearly indicate that the binding energy depends

ISSN 1512-1461

not only on the polarization charges but also on the ellipticity constant. Generally speaking all these work show that both size and geometry have a great influence on the optical properties of the systems.

In this preprint it is demonstrated how by varying the system's aspect ratio it is possible to reach significant modification of its properties giving rise to a very complicated spectrum. The study of the optical matrix elements in the dipole approximation shows interesting features induced by the dot shape.

Model and Theory

Within the framework of the effective mass approximation, the Schrödinger equation describing the motion of the electron trapped in EQD with a donor (acceptor) impurity reads

$$\left[-\frac{\hbar^2}{2m^*}\Delta_{XYZ}+V(X,Y,Z)\right]\Psi\left(X,Y,Z\right)=E\Psi\left(X,Y,Z\right) \qquad (1)$$

where m^* is the electronic effective mass.

Let's consider an ellipsoidal quantum dot with rotational symmetry around a given axis (the *Z* axis) with *c* major half-axes and *a* minor half-axes along the *Z* and *X*-*Y* directions, respectively. As a model of confining potential we consider the potential that is zero inside the ellipsoid and it is infinity outside

$$V\left(X,Y,Z\right)=\begin{cases}0, & \dfrac{X^2+Y^2}{a^2}+\dfrac{Z^2}{c^2}<1\\ \infty, & \dfrac{X^2+Y^2}{a^2}+\dfrac{Z^2}{c^2}\geq 1.\end{cases} \qquad (2)$$

As it was mentioned above such model is acceptable either for a quantum dot of a large volume or when the bandgap at the interface is sufficiently large. After following change of variables [8]

$$x\to\frac{a}{r_0}X,\quad y\to\frac{a}{r_0}Y,\quad z\to\frac{c}{r_0}Z;\quad r_0=\left(a^2c\right)^{1/3} \qquad (3)$$

the ellipsoid is transformed into sphere with reduced r_0 radius (without changing of QD volume). The Eq.(1) than can be rewritten in the following form

$$\left[-\frac{\hbar^2}{2m^*}\Delta_{xyz}+W(x,y,z)\right]\Psi\left(x,y,z\right)=E\Psi\left(x,y,z\right) \qquad (4)$$

with

$$W\left(X,Y,Z\right)=\begin{cases}\alpha\dfrac{\hbar^2}{2m^*}\left[\dfrac{c^2\left(a^2-r_0^2\right)}{r_0^2\left(c^2-a^2\right)}\Delta_{xyz}+\dfrac{\partial^2}{\partial z^2}\right], & x^2+y^2+z^2<r_0^2\\ \infty, & x^2+y^2+z^2\geq r_0^2\end{cases} \qquad (5)$$

Here $\alpha=r_0^2\left(c^2-a^2\right)\big/\left(ac\right)^2$ is the shape-anisotropy parameter that reflects the anisotropy of potential wall. If $\alpha<<1$ (i.e. ellipsoid is almost a sphere of radius r_0) the problem of finding the charge carrier (electron or hole) energy spectrum in an ellipsoidal quantum dot can be studied within the perturbation theory as a deformation with respect to the spherical dot.

The eigenfunctions and eigenvalues for unperturbed part $\hat{H}_0=-\hbar^2\Delta_{xyz}\big/2m^*$ correspond to states of particle in infinite spherical well. These eigenfunctions and eigenvalues are well known and can be found in any quantum-mechanical textbook [17].

ISSN 1512-1461

Result and Discussion

In order to calculate optical characteristics of EQD (Oscillator strength, OR coefficient) the knowledge of corresponding transition matrix elements are unavoidable. For this purpose in tern the knowledge of the system's eigenfunctions in it's initial and final states are necessary. These eigenfunctions and corresponding eigenenergies are obtained by means of perturbation theory and diagonalization method of Hamiltonian (the detail method of calculation can be found in [7] and in the references therein).

As it was shown in [7] the basic wavefunctions of the $\hat{H}_0$ unperturbed Hamiltonian are not bound and hence the states with even (*g*) and odd (*u*) parity can be considered independently. Introducing the ellipsoid aspect ratio by $\chi = c/a$ (only $\chi > 1$ for prolate ellipsoid is considered in this preprint) prolate ellipsoid quantum dot spectrum as a function of χ is shown in Fig.1 (in units of $2m^* E_{nlm} r_0^2 / \hbar^2$). $E_{nlm} = (\hbar^2 / 2m^* c^2)\,\beta(\chi)$ where $\beta(\chi)$ is an adimensional quantity depending just on the ellipsoid aspect ratio but not on *a* or/and *c* separately.

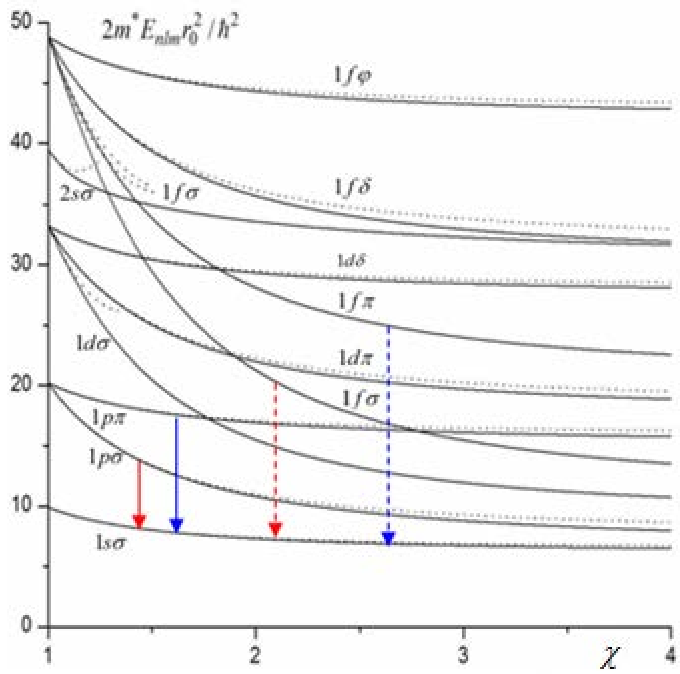

Figure 1: The prolate ellipsoidal nanoparticle spectrum as a function of χ. The energies are calculated with $a = r_0 = 1$ nm. The solid and dotted curves show the results of calculations by use of method of diagonalization of Hamiltonian and perturbation treatment respectively. The curves notations and arrow indications are given in text.

Here $n = 0,1,2...$, $m = 0,\pm1,..,$ $l = |m|,|m|+1,...$ in analogy to the SQD. Designations $s, p, d, f...$ and $\sigma, \pi, \delta, \varphi...$ are borrowed from atomic orbital classification and diatomic molecular theory and denotes the energy levels with $l = 0,1,2...$ and $|m| = 0,1,2...$ respectively [18] (Strictly speaking this orbital classifications are correct only when $\chi = 1$ i.e. in spherically symmetrical case, but it is kept also when $\chi > 1$ in order to follow the origin of the each anisotropic state). In Hamiltonian diagonalization method this anisotropic states can be represented as a linear combinations (mixing) of basic spherically symmetrical eigenfunctions of $\hat{H}_0$ unperturbed Hamiltonian. In this work only

ISSN 1512-1461

two lower even states $|1s0\rangle, |1d0\rangle$ and two lower odd states $|1pm\rangle, |1fm\rangle$ are used for construction of the EQD's states. The lower degree of symmetry of EQD with respect of SQD relaxes the typical selection rule $\Delta l = \pm 1$ making in principle allowed any transitions for which Δl is odd. In this case allowed transitions to the ground $|100\rangle$ state are $|nlm\rangle \to |100\rangle$ with $l = 1, 3, 5...$ and $|m| = 0,1$ [6]. Transition with $\Delta m = 0$ involve radiation linearly polarized along the z axis, while transition with $\Delta m = \pm 1$ radiation circularly polarized in *x-y* plane.

The dipole matrix elements have been calculated for transitions $|110\rangle \to |100\rangle$ (red solid arrow in Fig.1) $|130\rangle \to |100\rangle$ (blue solid arrow in Fig.1) corresponding linearly polarized radiation along the z axis and $|111\rangle \to |100\rangle$ (red dashed arrow in Fig.1) $|131\rangle \to |100\rangle$ (blue dashed arrow in Fig.1) corresponding circularly polarized radiation along the *x-y* plane. The results are presented in Fig.2

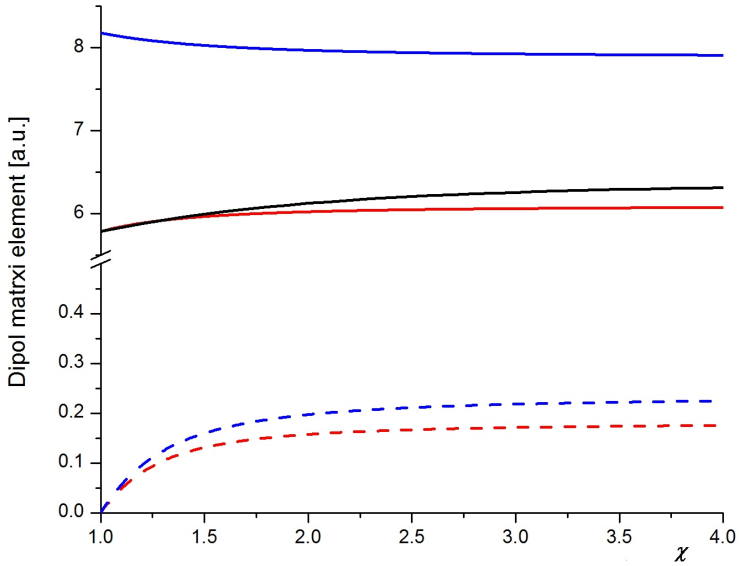

Figure 2: The dipole transition matrix element a function of χ. $a = r_0 = 1$ nm. Red solid curve $|110\rangle \to |100\rangle$ transition; red dashed curve $|111\rangle \to |100\rangle$ transition; blue solid curve $|130\rangle \to |100\rangle$ transition; blue dashed curve $|131\rangle \to |100\rangle$ transition. The black solid curve $|110\rangle \to |100\rangle$ calculated by use of first order perturbation theory.

The analysis of Fig.2 gives clear evidence to the fact that by realizing anisotropic systems, polarization dependent processes can be obtained. The more the dot geometry is different from the spherical one the more 'anisotropic' is its response to polarized radiation.

Conclusion

In this work optical properties of ellipsoidal quantum dots have been discussed. From all these preliminary results, it comes out that the fabrication of shape-controlled ellipsoid quantum dots can have fundamental applications. The consideration of different confined potentials (parabolic or finite heights wall) are highly desired.

ISSN 1512-1461

Acknowledgments

The work is supported by Shota Rustaveli National Science Foundation under grant # DI/27/6-265/13

References:

1. W. Wegscheider, G. Schedelbeck, M. Bichler and G. Abstreiter, *Physica* E (1998) **3,** 103
2. Lei Zhuang, Guo Lingjie and S. Y. Chou, *Appl. Phys. Lett.* (1998) **72,** 1205
3. M. Grundmann, *Physica* E (2000) **5,** 167
4. G. Cantele, D. Nino, G. Iadonisi, J. Phys. Condens. Matter (2000) **12,** 9019
5. G. Cantele, D. Ninno, and G. Iadonisi, Nano Lett. (2001) **1,** 121
6. G. Cantele, D. Ninno, and G. Iadonisi, Phys. Rev. B (2002) **64**, 125325
7. T. Kereselidze, T. Chelidze, R. Ya. Kezerashvili, Physica E (2015) **68**, 65
8. K.G. Dvoyan, E.M. Kazaryana, L.S. Petrosyan, Physica E, (2005) **28** 333
9. V.I. Boichuk, V.B. Hol’skyi, R.YU. Kubay, R.I. Lukin, Ukr. J. Phys., (2008) **53** 574
10. V.P. Dzyuba, Yu. N. Kulchin, V.A. Milichko, Physics of the Solid State, (2014) **56** 359
11. W.F. Xie Physica B (2010) **405** 3436
12. W.F. Xie, Journal of Luminescence (2011) **131** 943
13. K.X. Guo, S.W. Gu, Physical Review B (1993) **47,** 16322
14. E. Sadeghi, Superlattices and Microstuctures (2011) **50,** 331
15. G. Rezaei, M.R.K. Vahdani, B. Vaseghi, Current Applied Physics (2011) **11,** 176
16. E. Sadeghi, F. Vahdatnejad, M. Moradi L.M, Superlattices and Microstructures (2013) **58** 165
17. B. H. Bransden, C. J. Joachain, Quantum mechanics (2nd ed.). (Essex: Pearson Education 2000) p 457
18. L.D.Landau, E.M. Lifshitz, Quantum Mechanics: Non-Relativistic Theory, (Elsevier, Singapore, 2007) p 330

Article received on: 2016-05-11