

LAYERED NANOSTRUCTURES

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Summary

Semiconductor quantum dots are unique nanostructures in which the effects of size-quantization are the most highlighted. Due to the full quantization of the spectrum of the charge carriers, which are in quantum dots, the physical characteristics of quantum dots have much in common with atoms. As of today, different geometrical forms and sizes of quantum dots are realized, in which there is a possibility to realize strong manipulation of energetic spectrum, thereby the physical characteristics of the examined systems.

An interesting class of zero-dimensional systems is layered spherical and cylindrical quantum dots, as well as quantum rings. In the systems like these, the radial motion of the charge carriers are limited both in the inner and outer borders. The mentioned reason allows even the simplest – spherical symmetry case to control the spectrum of the charge carriers with the help of two geometrical parameters: inner and outer radii.

Also, we should especially mention, that the theoretical results gained through the research of physical characteristics of layered nanostructures have generalizing character, as by the corresponding limiting process both quantum wells and quantum wires can be realized.

1. Introduction

While describing the behavior of microparticles, and particularly electron, it is necessary to clarify whether to describe it in the frameworks of classical or quantum theory. It is well known that quantum effects demonstrate themselves in the case when the effective area of the localization of particle is comparable with its de Broglie wavelength. De Broglie wavelength is defined according to the formula:

$$\lambda_D = \frac{2\pi\hbar}{m_0v} \quad (1)$$

where m_0 is the mass of the free particle, v is its velocity. For the electron at room temperature $\lambda_D \sim 10^{-8}$ cm and especially for that reason the theory of hydrogen atom is purely quantum – the area of the localization of electron is about Bohr radius the value of which is also about 10^{-8} cm.

While describing the semiconductor state on the base of detailed calculations it appears that due to translational symmetry of crystal lattice, the behavior of electron can be considered as a free motion, not with the mass of free electron, but with certain effective mass μ . Considering that in the semiconductor compounds of type A^3B^5 , such as *GaAs* or *InSb*, $\mu \ll m_0$ ($\mu(\text{GaAs}) = 0,067m_0$, $\mu(\text{InSb}) = 0,015m_0$) instead of common de Broil wave it is necessary to insert the length of effective de Broil wave

$$\lambda_D^* = \frac{2\pi\hbar}{\mu v} \quad (2)$$

Because of the smallness of the value of effective mass the following inequality takes place

$$\lambda_D \ll \lambda_D^* \quad (3)$$

from which follows that quantum effects in semiconductor structures show themselves during the localization of charge carriers (CC) in the area of order of hundreds of angstrom. In other words, if the sizes of semiconductor in any direction or several directions are comparable with the effective value of electron de Broil wave, then it is necessary to apply the quantum mechanical description of the behavior of particles by considering the availability of walls in the mentioned direction (directions). The existence of the borders in the semiconductor structure is considered by inserting a confinement potential on the heterojunction of the considered semiconductor and environment. As far as the quantization of the energetic levels of CC depends on the sizes of a semiconductor, then that type of quantization is accepted to call size quantization. Quantum size effects are more brightly expressed in zero-dimensional structures, or, in other words, in quantum dots (QD). In such systems the energetic spectrum of CC becomes totally quantized. Due to the total quantization of the energy of CC in QDs its characteristics become similar in great deal with those that are inherent

to the real atoms that is why they are often called “artificial atoms”. Nowadays, due to the modern methods of growing semiconductor nanostructures spherical, cylindrical, ellipsoidal, pyramidal, lens-shaped and other QDs are experimentally realized. It is evident, that in such palette of zero-dimensional systems on the one hand general properties are inherent, on the other hand – strictly specific ones, that are dictated both with the geometry of a certain shape, and composition of its components. It is remarkable, that from the point of view of the theoretical description of physical processes in QDs on the first stage of the investigation an important task becomes the problem of construction of more realistic Hamiltonian of the studied system as much as possible. Consideration of the effect of the size-quantization in Hamiltonian is carried out by inserting the interaction potential of CC with the walls of QDs. There with if the physicochemical characteristics of QDs and the environment form the height and the profile of the confinement potential, then its geometry defines the symmetry of Hamiltonian, hence, also the degree of degeneracy of levels of CC.

Different authors have discussed different models of confinement potentials of QDs:

- Infinite high rectangular potential
- Rectangular potential of finite height
- Parabolic confinement potential
- Hulthen potential
- Pöschl-Teller potential, etc.

On the choice of corresponding confinement potential can influence for example such factors as interdiffusion of QD component and environment in the process of the growth of a sample, the degree of difference of QD lattice constant and environment. The choice of a correct mathematical model of the confinement potential can be determined by comparing the theoretical results with the data of the experiment. A bright example of a successful theoretical proof of the results of an experiment, by choosing a correct confinement potential, is the experimental detection and the theoretical proof of generalization of Kohn theorem for QDs.

2. Layered Nanostructures with the Simplest Geometry

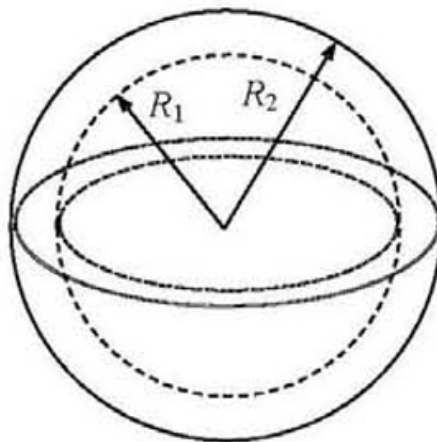


Figure 1. Spherical nanolayer

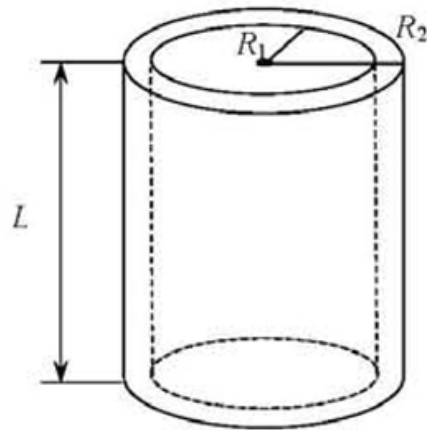


Figure 2. Cylindrical nanolayer

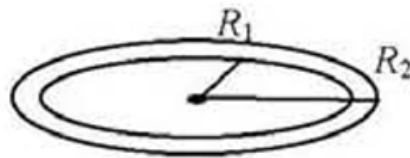


Figure 3. Quantum ring

During the last decade the interest has greatly grown towards QDs having layered and particularly towards the ring-shaped ones. An important peculiarity of such systems is the presence of transition of both outer and inner borders from QDs to the environment. Spherical and cylindrical layered QDs as well as two-dimensional quantum rings have simpler geometrical form. Schematically those systems are presented on the Figures 1, 2, 3.

The results obtained during theoretical research of physical characteristics of layered structures have general character, as far as in proceeding to the limit the corresponding layered QDs can transform not only to quantum wire and quantum wells, but also to QDs with simpler geometry. Let us discuss it on the example of a cylindrical nanolayer. From figure 2 follows that:

1. not changing the height of the layer L and in proceeding to the limit $R_1 \rightarrow 0$, and also $R_2 \rightarrow \infty$ we will come to the case of quantum wells,
2. not changing the outer radius R_2 and in proceeding to the limit $R_1 \rightarrow 0$, and also $L \rightarrow \infty$ we will come to the case of quantum wires,

3. not changing the outer radius R_2 and also the height of the layer L and in proceeding to the limit $R_1 \rightarrow 0$ we will come to the case with cylindrical QDs.

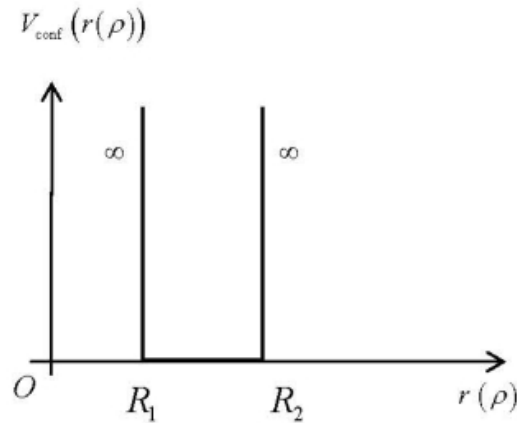


Figure 4. Rectangular infinite high confinement potential of spherical (cylindrical) nanolayer. The electron is localized in the area between R_1 and R_2 .

For describing the above mentioned layered nanostructures the necessity occurs to construct the confinement potential taking into account the geometrical specificity of studied instances. It is clear that the confinement potentials, depending on the studied case (spherical or cylindrical nanolayer), will have either spherical or cylindrical symmetries. Concerning to the behavior of these potentials on the radial direction, then their forms are mostly defined with the methods of growth of certain samples and also the specificity of the components of sample and the environment. In a simple approximation the confinement potential of nanolayer or of quantum ring can be presented in the frameworks of a model of two-dimensional, as well as three dimensional rectangular quantum well of infinite height (Figure 4). These models assume that wavefunction becomes zero on the inner (circle or a sphere with radius R_1) and outer (circle or a sphere with radius R_2) borders of QD.

The symmetry of the mentioned systems makes their theoretical description more optimal not in Cartesian coordinate system, but in spherical and cylindrical coordinate systems. Meanwhile, the location of a point in space in spherical coordinates is defined with the help of three-dimensional radius r and two angles: zenithal θ and azimuthal φ (Figure 5). From Figure 5 the dependence between Cartesian and spherical coordinates is followed:

$$\left. \begin{aligned} x &= r \sin \theta \cos \varphi \\ y &= r \sin \theta \sin \varphi \\ z &= r \cos \theta \\ r &= \sqrt{x^2 + y^2 + z^2} \end{aligned} \right\} \quad (4)$$

In cylindrical coordinate system the location of a point in space is defined with the help of two-dimensional radius ρ , azimuthal angle φ and coordinate z (Figure 6). Analogically with the help of Figure 6 the dependence between the sets of coordinates $\{x, y, z\}$ and $\{\rho, \varphi, z\}$ can be found:

$$\left. \begin{aligned} x &= \rho \cos \varphi \\ y &= \rho \sin \varphi \\ z &= z \\ \rho &= \sqrt{x^2 + y^2} \end{aligned} \right\} \quad (5)$$

The behavior of particles in nanolayers needs to be described with Schrödinger equation which has the following form for the stationary (independent upon time) fields:

$$-\frac{\hbar^2}{2\mu} \Delta_{x,y,z} \Psi(x, y, z) + V_{\text{conf}}(x, y, z) \Psi(x, y, z) = E \Psi(x, y, z), \quad (6)$$

where $V_{\text{conf}}(x, y, z)$ – characterizes the potential energy of particles, $\Delta_{x,y,z}$ – is the Laplace operator in Cartesian coordinates having the form of:

$$\Delta_{x,y,z} = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \quad (7)$$

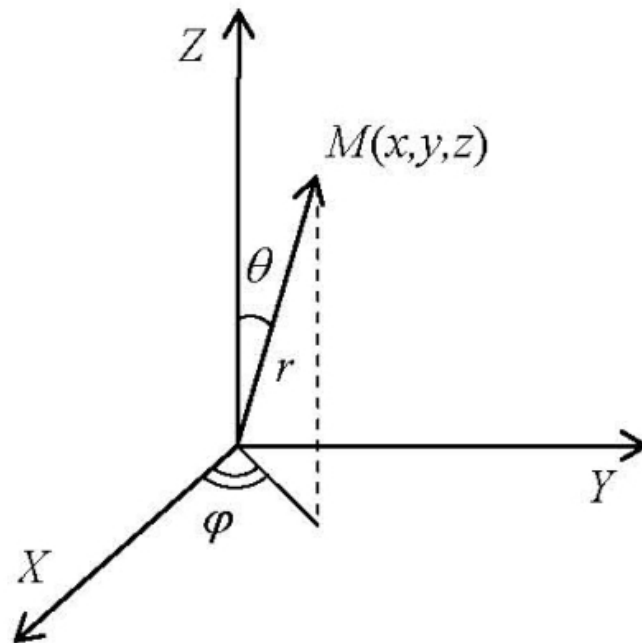


Figure 5. Spherical coordinate system.

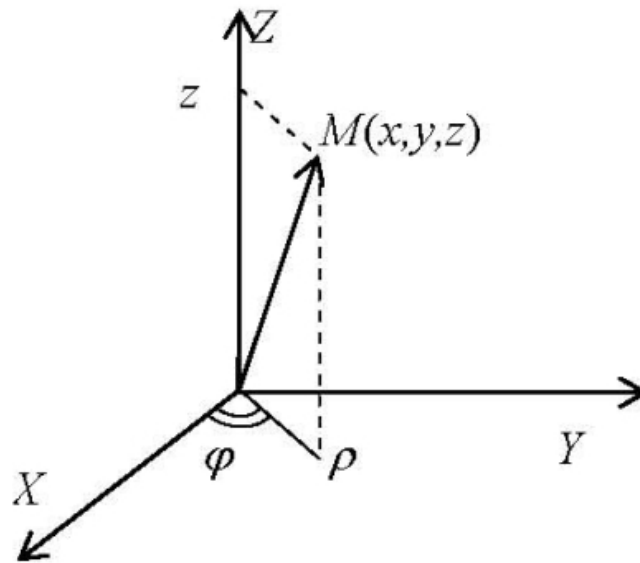


Figure 6. Cylindrical coordinate system.

During describing the behavior of CC in spherical and cylindrical nanolayers the physical pictures becomes more transparent if we represent the potential energy of interaction between particle and walls of QD accordingly in spherical and cylindrical coordinates. For this reason there is a necessity to write down the Schrödinger equation in the mentioned coordinate systems. By not going into the details of mathematical transformations, we should mention that for both cases the Schrödinger equation has to be written by considering the form of the Laplace operator in spherical $\Delta_{r,\theta,\varphi}$ and cylindrical $\Delta_{\rho,\varphi,z}$ coordinates. With the methods of mathematical physics it is obtained that for both cases the angular and radial motions can be separated from each other. Meanwhile, angular wave functions are represented with well known polynomials and exponential functions, independent of the form of both spherical and cylindrical symmetrical fields.

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Biographical Sketch

Eduard Kazaryan – Deputy Rector of Russian-Armenian (Slavonic) University, head of the chair of general and theoretical physics of the department of physics and technology, doctor of physical and mathematical sciences, professor. In 1965 he graduated from Moscow State University. In 1971 he defended his candidate's dissertation and in 1981 his doctoral dissertation. In 1983 he got the title of professor. In 1996 Eduard Kazaryan was elected as a member of National Academy of Sciences of Armenia. The researches are devoted to the solid state physics, excitonic physics, the physics of low-dimensional semiconductor systems. He is the co-author of monograph “Physical bases of Nanoelectronics” (in 2005, in Armenian). Author of more than 140 articles devoted to the above-mentioned topics. In 2008 was awarded by the prize of President of Republic of Armenia in the field of physics for the series of papers on the theory of electronic and optical properties of nanostructures.

Hayk Sarkisyan – Dean of the department of physics and technology of Russian-Armenian (Slavonic) University, doctor of physical and mathematical sciences, professor of the chair of general and theoretical physics. In 1994 he graduated from Yerevan State University. In 1997 he defended candidate's dissertation and in 2005 his doctoral dissertation. The field of scientific interests refers to the theory of electronic and optical properties of nanostructures. The researches are devoted to the theory of excitonic and impurity states, as well as optical absorption in quantum wells, wires and dots on the one hand with the presence of external fields, and on the other hand – accounting the non-parabolic dispersion law of charge carriers. Hayk Sarkisyan is the author of more than 50 articles devoted to the mentioned topic. In 2008 was awarded by the prize of President of Republic of Armenia in the field of physics for the series of papers on theory of electronic and optical properties of nanostructures.