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The effect of magnetic field and donor impurity on electron spectrum in spherical core-shell quantum dot

V.A. Holovatsky*, O.M. Voitsekhivska, M. Ya Yakhnevych

Chernivtsi National University, Kotsiubynsky Str., 2, 58012, Chernivtsi, Ukraine

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ABSTRACT

The effect of homogeneous magnetic field and location of donor impurity on the electron energy spectrum and distribution of its probability density in spherical core-shell quantum dot is investigated. In the framework of the effective mass approximation and rectangular infinitely deep potential well, the solutions of the Schrodinger equation are found using the matrix method. The wave functions are expanded over the complete set of exact functions obtained without the magnetic field and impurity.

It is shown that when the induction of magnetic field increases, the ground state of electron in the nanostructure without impurity or on-center impurity is successively formed by the states with m = 0, −1, −2, … (Aharonov-Bohm effect). When donor impurity is located in the shell of the nanostructure the Aharonov-Bohm effect vanishes.

The dependences of electron energy spectrum and its wave functions on the location of impurity, placed along the direction of magnetic field or perpendicularly to it, are studied. It is shown, that in the first case, the quantum states are characterized by the certain value of magnetic quantum number *m* and the expansion contains the wave functions of the states with it only. In the second case, the cylindrical symmetry of the problem is broken and the new quantum states are formed from the states with different values of all three quantum numbers *n*, *l*, *m* and electron energy spectrum weakly depends on the magnetic field induction.

1. Introduction

Quantum dots (QDs) of different sizes, shapes and compositions have been intensively investigated during last two decades. Recently, the new technological methods have been developed in order to grow the simple semiconductor QDs and multilayered spherical QDs with complicated radial structure, forming the specific profiles of potential energies for electron and hole which are necessary for the practical use. These nanostructures are differently called: quantum dot quantum well (QDQW), core-shell QD, core-shell-shell QD, onion-like QD and so on [1–10]. The majority of theoretical studies are performed in the framework of the effective mass approximation and the model of rectangular potential barriers for the nanostructures with different symmetry [6–11]. Using them, one can exactly solve the Schrodinger equation for the simple structure and, further, research the interactions between quasi-particles, as well as with external fields and impurities.

* Corresponding author.
E-mail address: ktf@chnu.edu.ua (V.A. Holovatsky).

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The optical properties of multilayered nanostructures with central Coulomb impurity are studied in refs. [12] using the exact solutions of Schrodinger equation. When the impurity is off-center, the Schrodinger equation cannot be solved exactly, thus the electron spectrum is obtained within variational [6–23] and perturbation method [16]. In Ref. [14], the energy of electron ground state is calculated in order to study its binding energy with donor impurity in single QD GaAs/$Ga_{1-x}Al_xAs$. The problem becomes more difficult when the interaction between electron and impurity is studied for the multilayered nanostructures.

For instance, in Ref. [15], the energies of electron and hole in ground states are calculated and the oscillator strengths of interband quantum transitions are analyzed for multilayered nanostructures ZnS/CdS/SiO_2 and CdS/ZnS/CdS/SiO_2. In order to study the intraband transitions, one has to know the wave functions of the excited states. Their calculation within the variational method meets a problem of the correct trial functions, which should satisfy the orthogonality conditions for all states. Thus, only two or three exited states are usually studied by means of this method. In ref. [18], the authors compared the results for the ground and exited electron states in nanostructure CdS/SiO_2 obtained within the variational method with that of the method of expansion of electron wave functions in structure with off-center impurity over the exact wave functions in QD with central impurity. The second method gave opportunity to get the necessary number of exited states in order to research the optical properties of nanostructure. The electron energy spectrum obtained within the expansion method with good accuracy correlate with result of variational method. In Ref. [22], the binding energy of electron with off-center donor impurity in ellipsoidal QD is studied using the expansion method in the framework of parabolic potential model. During the last years, this method is often used in order to research the effect of external fields on the energy spectra of quasi-particles in spherical nanostructures [24–30]. It allows obtaining the complete energy spectrum of quasi-particles, while the expansion coefficients determine the partial contribution of the states of the non-perturbed system in obtained solutions. Therefore, expansion method is better than the direct numerical method of the solution of Schrodinger equation, for example, finite element method (FEM) [31,32] or Runge −Kutta method [33]. In papers [24–30], the expansion method is used for the spherically symmetrical nanostructures, in which the perturbation transforms the spherical symmetry of the problem into the cylindrical one. In this case, the quasi-particle state is characterized by the certain value of the magnetic quantum number and expansion is performed only over the states with different values of n and l quantum numbers. The obtained energies and wave functions of electron allowed calculation of the oscillator strengths of all most probable intraband quantum transitions and research the effect of the external fields.

The effect of magnetic field on the ground and exited states of electron studied for spherical nanostructure, ref [25,26,34], proved that the energy of the states with $m < 0$ at first decreased when magnetic field induction increased, taking into account its linear term, reached minimum and further increased due to the square term. According to such non-monotonous dependence, the ground state was successively formed by the states with $m = 0, -1, -2, \ldots$ Herein, the magnetic quantum number of the ground state changes step-like when magnetic field intensity increases by the same magnitude (Aharonov-Bohm effect), ref. [25,26,34].

The results of research of joint effect of electric and magnetic fields on electron spectrum in spherical layer, ref. [25], prove that at the certain intensity of electric field even when magnetic field is strong, the state with $m = 0$ becomes again the ground one, i. e. the Aharonov-Bohm effect is broken. The influence of the impurity position on the formation of electron ground state in spherical structures driven by strong magnetic field is not studied yet. The first attempts were performed in Ref. [19], where the magneto-optical properties of AlAs/GaAs/SiO_2 nanostructure were investigated within the variational method. According to the physical considerations, the variational functions were constructed for the ground and exited states and the absorption coefficient of quantum transition $1s \rightarrow 1p_z$ was calculated. Considerable difficulties arise when the other excited states, particularly with $m < 0$, are observed within the variational method.

In this paper, we study the joint effect of homogeneous magnetic field and donor impurity on electron energy spectrum in spherical core-shell nanostructure. Two cases of different location of impurity with respect to the direction field and the center of nanostructure are observed.

2. The scrodinger equation for the electron in spherical core-shell nanostructure driven by magnetic field

We consider the multilayered spherical nanostructure which consists of the core ZnS − potential barrier ($r < r_1$), spherical shell CdSe − potential well ($r_1 \le r \le r_2$) and semiconductor matrix ZnS ($r > r_2$). The coordinate system is chosen so that its origin coincides with QD center and OZ axis − with the direction of magnetic field induction. Two different locations of donor impurity are observed: if it is placed on OZ axis, the problem has the cylindrical symmetry and if it placed on OX axis, this symmetry is broken.

Taking into account the high potential barriers at the structure interfaces ($V_e = 1.05$ eB, ref. [32]), the problem is solved in the framework of infinitely deeply rectangular potential well. Herein, the Schrodinger equation for an electron in spherical nanostructure has the form

$$\frac{1}{2\mu}\left(\vec{p} - \frac{e}{c}\vec{A}\right)^2 \Psi_f(\vec{r}) + \left[U(r) - \frac{Z e^2}{\varepsilon\left|\vec{r} - \vec{r}_{imp}\right|}\right]\Psi_f(\vec{r}) = E_f \Psi_f(\vec{r}) \tag{1}$$

where