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Effect of Electric Field on Energy Spectrum and Intersubband Absorption Coefficient of Electron in Spherical Multilayered Quantum dot CdSe/ZnS/CdSe

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In this paper, the energy spectrum of electron and complete set of exact wave functions are obtained in the framework of effective mass approximation and rectangular potential barriers model for the CdSe/ZnS/CdSe nanostructure. Using the matrix method, the numeric calculations are performed for the electron energy spectrum as a function of electric field strength in multilayered quantum dot. It is shown that the electric field effects on the core electron in the ground state and causes its tunneling into the outer potential well. Thus, the overlap of wave functions varies essentially, influencing the dipole momentum of quantum transitions and light absorption coefficient.

Keywords: QDQW, multilayered QD, intersubband absorption, intraband transitions.

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Introduction

Semiconductor spherical quantum dots are intensively studied since last century because these nanostructures are the basic elements of new devices of nano- and optoelectronics. The first multilayered nanostructure CdS/HgS/CdS, the so called QDQW, was grown in 1993 by Mews and others [1-2]. Later, the spherical nanostructures based on CdS, CdSe, ZnS, ZnSe and other semiconductor crystals [3-7] have been synthesized. High-efficiency LEDs, white light sources, photodetectors, fluorescent labels, single-electron devices for computer engineering, biological sensors and so on are produced using the multilayered QDs. The wide perspectives of their practical utilization stimulate the intensive theoretical researches of their optical properties. In the majority of theoretical studies the effective mass approximation and model of rectangular potential wells and barriers [8-9] are used. The electron energy spectrum and analytical form of its wave functions were obtained in papers [8-9]. The sizes of potential wells were chosen in such a way that if the electron was located in outer well, the field pushed it into the inner one. Such change of electron location was displayed by the optical properties.

In this paper, the energy spectrum of electron and complete set of exact wave functions are obtained in the framework of effective mass approximation and rectangular potential barriers model for the CdSe/ZnS/CdSe nanostructure. Using the matrix method, the numerical calculations are performed for the electron energy spectrum as function of electric field in multilayered quantum dot. The polarization potentials, arising from the difference of dielectric constants values in different layers of nanostructure and external medium are taken into account.

It is shown that the effect of electric field on the core electron in the ground state causes its tunneling into the outer potential well. Thus, the overlap of wave functions is essentially varied, that influences on the dipole momentum of quantum transitions and light absorption coefficient.

I. Theoretical model

The semiconductor spherical QDQW consisting of core-well with the radius r_0, barrier with the thickness $\Delta = r_1 - r_0$ and well with the width $r = r_2 - r_1$ placed into the semiconductor matrix-barrier is studied. In order to investigate the effect electric field on the electron energy spectrum and wave functions in the nanostructure with an impurity, the Schrodinger equation with the Hamiltonian

$$H = \hat{\nabla}\frac{\hbar^2}{2m(r)}\hat{\nabla} + V_E(r,q) + W(r) + U(r) \qquad (1)$$

is to be solved. Here $V_E(\mathbf{r})$ is electrostatic potential of the external field $\mathbf{F}$, applied in z-direction, has the form

$$V_E(r,q) = -eF\cos q \begin{cases} a_0 r, & r \le r_0 \\ a_1 r + \dfrac{b_1}{r^2}, & r_0 < r \le r_1 \\ a_2 r + \dfrac{b_2}{r^2}, & r_1 < r \le r_2 \\ r + \dfrac{b_3}{r^2}, & r > r_2 \end{cases} \quad (2)$$

The coefficients a_i and b_i are obtained as solutions of Poisson equation with standard dielectric boundary conditions at the interfaces. The $W(r)$ term in (1) describes the electron self-polarization potential, which for the case of a small difference between e_w and e_b is simplified to the following form [9]

$$W(r) = \frac{e^2(e-e_m)}{8pe\, r_2} \sum_{k=0}^{\infty} \frac{k+1}{k e + (k+1)e_m} (r/r_2)^{2k}, \quad (3)$$

Confining potential $U(r)$ and effective mass $m(r)$ have a step-wise form:

$$U(r) = \begin{cases} 0, & r \le r_0,\ r_1 < r \le r_2 \\ V, & r_0 < r \le r_1 \\ \infty, & r > r_2 \end{cases} \quad (4)$$

$$m(r) = \begin{cases} m_0, & r \le r_0,\ r_1 < r \le r_2,\ \textit{wells} \\ m_1, & r_0 < r \le r_1,\ \textit{barrier}. \end{cases} \quad (5)$$

If $B = 0$, $E = 0$, the Schrödinger equation with Hamiltonian (1) has the exact solutions

$$\Phi_{nlm}(r,q,j) = R_{nl}(r) Y_{lm}(q,j), \quad (6)$$

where $R_{nl}(r) = A_{nl} j_l(k_{nl} r) + B_{nl} n_l(k_{nl} r)$ with $j_l(z)$, $n_l(z)$ being the Bessel spherical functions of the first and the second kind, respectively.

In order to study the electron properties in nanostructure driven by electric and magnetic fields, we use the method of expansion of the quasi-particle wave function over the complete set of eigen functions for the electron in the spherical nano-structure without the external field, obtained as the exact solutions of Schrödinger equation. When the external fields are applied, the spherical symmetry of the problem is broken and the orbital quantum number l appears to be an inconvenient one. The new states characterized by a magnetic quantum number m are represented as a linear combination of the states $|nlm\rangle$

$$y_{jm}(\mathbf{r}) = \sum_n \sum_l c_{nl} \Phi_{nlm}(\mathbf{r}), \quad (7)$$

Substituting (8) into Schrödinger equation with Hamiltonian (1), we obtain the secular equation

$$\left| H_{nl,n'l'} - E_{jm} d_{n,n'} d_{l,l'} \right| = 0. \quad (8)$$

The problem of electron energy spectrum and wave functions calculation under the external fields and impurity effect is solved, eigenvalues and eigenvectors of the matrix are obtained.

The calculations of absorption coefficient are performed [11-15] using the formula:

$$a(w) = w\sqrt{\frac{m_0}{e_0 e}} \sum_{i,j} \sum_{a,b} \frac{s \left| M_{ia,jb} \right|^2 \mathbf{h}\Gamma_{ia,jb}}{\left(E_j - E_i - \mathbf{h}w\right)^2 + \left(\mathbf{h}\Gamma_{ia,jb}\right)^2}, \quad (9)$$

where e_0 is electric vacuum constant, m_0 stands for magnetic constant, c represents the speed of light, $\mathbf{h}\Gamma_{1,2}$ is energy of relaxation. Dipole momentum of quantum transition, in its turn, is given by the formula:

$$M_{i-f} = \left| \langle i | \sqrt{m(r)}\, r \cos q \mid f \rangle \right|^2, \quad (10)$$

II. Results and discussion

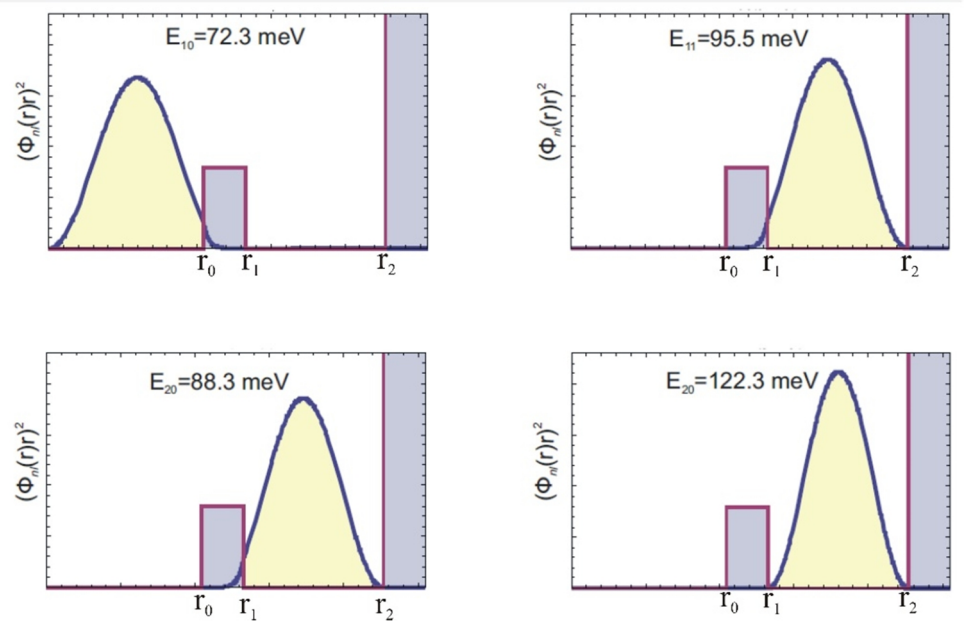

Fig. 1. Theradialdistributionofprobabilitydensityattheelectronenergystates |10>, |11>, |20>and |21>.

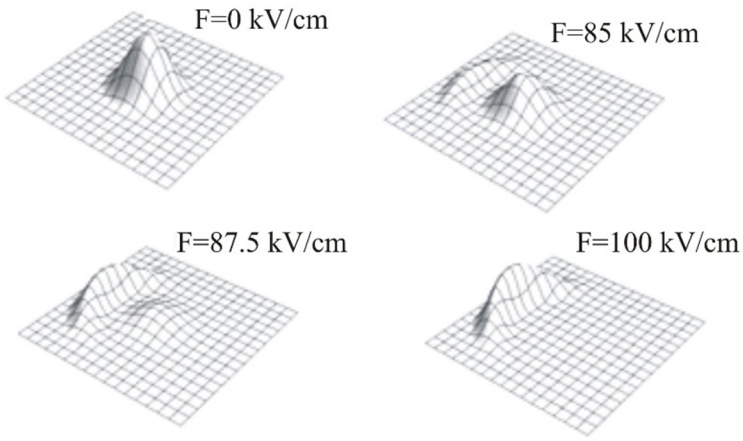

Fig. 2. Distribution of electron density in the ground state in nanosystem at different values of electric field strength.

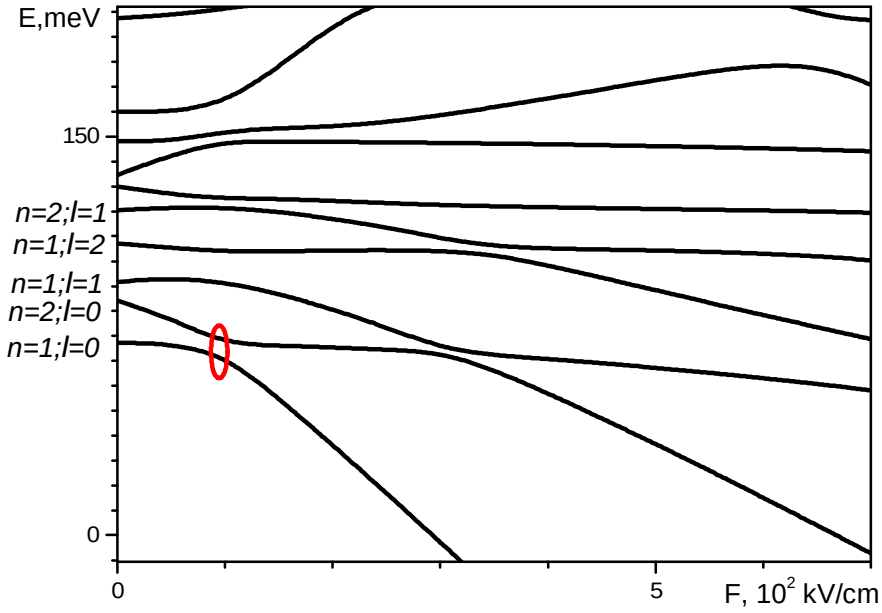

Fig. 3. Electron energy spectrum as function of electric field strength in nanostructure. Anti-crossing is high lighted in red.

The computer calculations were performed using the physical parameters of CdSe/ZnS/CdSe semiconductor: $m_0^e = 0.13 m_e$, $m_1^e = 0.28\, m_e$, $V = 1050\, meV$, $e_w = 9.3$, $e_b = 8.1$, $e_m = 1$, where m_e denotes a bare electron mass. The potential wells sizes are chosen in such a way that electron is localized in the core of nanostructure without electric field (r_0=5.5*nm*, r=5*nm*, Δ=1.5 *nm*). All calculations are performed at m=0. In fig. 1 the radial distribution of probability density for electron in the ground and first three existed states are presented. We took into account no less than 36 terms in the expansion (8) (n=1,...,6 and l=0,...,5).

The results of calculations for $|y_{10}(\mathbf{r})|^2$ show (see fig. 2), that the electron, at geometric parameters choosen, is located in the core of nanostructure. From the fig. 2 it is clear that the electron tunnels into outer well at 83 – 88 kV/cm. It is also manifested in the dipole momentum, oscillator's strength and absorption coefficient.

The dependences of several lower energy levels of electron on the electric field strength F are shown in fig. 3. Here one can see that change of electron location is accompanied by the effect of anticrossing energy levels. The energy of ground state of electron, which is located in outer potential well, linearly decreases after anti-crossing at increasing electric field.

We calculated the absorption coefficient at different values of electric field intensity. The selection rules for intraband quantum transitions of the electron in QDQW without electric field are defined by the integral of the product of the wave functions over the angular variables. It is nonzero for the transitions with $\Delta l = \pm 1; \Delta m = 0$.

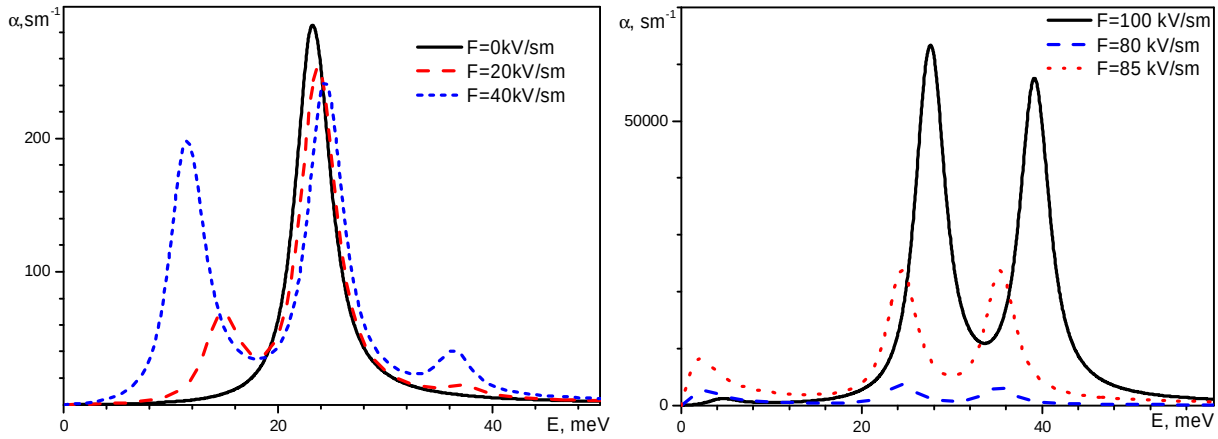

Fig. 4. Absorption coefficients for intersubband quantum transitions at different values of electric field strength.

Thus, the transitions from the ground state are possible only into the states with $l = 1$. From the fig.4 one can see that the transition |1>→|3> is permitted when the electric field is absent. When the electric field strength increases, the probability of transitions |1>→|2> and |1>→|4> increases too, together with the value of absorption coefficient. Comparing the results one finds that the absorption coefficient at 80 kV/cm is much bigger than that at 40 kV/cm. Increasing intensity of electric field causes larger oscillator strength of these transitions. The properties of electron energy spectrum in the nanostructure under study can be implemented in new semiconductor devices.

Summary

In order to obtain the electron energy spectrum and its density distributions in semiconductor QDQW driven by electric field, the stationary Schrodinger equation is solved within the method of wave function expansion over the basis of electron wave functions obtained for the nanostructure without the external field. The approximation of effective mass and finite rectangular potential barriers model are used. The dependences of electron energies, density distributions and absorption coefficient on electric field intensity are obtained. It is shown that the electric field dramatically changes the electron density distribution. When the electron, in ground state, is located in the core of the QDQW potential well, the increasing electric field intensity causes its tunneling into outer potential well.

The optical properties of the QDQW depend on the distribution of electron density in spherically-symmetric states, varying due to the electric field. This phenomenon can be used for the creation of new semiconductor nanodevices operating in the infrared range of electromagnetic waves.

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Вплив електричного поля на енергетичний спектр та міжпідзонний коефіцієнт поглинання електрона в сферичній багатошаровій квантовій точці CdSe/ZnS/CdSe

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Енергетичний спектр електрона і повний набір хвильових функцій знайдено в моделі наближення ефективних мас та прямокутних потенціальних бар'єрів в наноструктурі CdSe/ZnS/CdSe. Використовуючи матричний метод розраховано енергетичний спектр електрона в багатошаровій квантовій точці, як функцію напруженості електричного поля. Показано, що вплив електричного поля на електрон, який локалізований в ядрі наносистеми в основному стані спричиняє тунелювання в зовнішню потенціальну яму. Це відображається на перекритті хвильових функцій, дипольних моментах квантових переходів і коефіцієнті поглинання.