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Original paper

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ENERGY LEVELS OF AN ELECTRON IN A CIRCULAR QUANTUM DOT IN THE PRESENCE OF SPIN-ORBIT INTERACTIONS

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Abstract. The two-dimensional circular quantum dot in a double semiconductor heterostructure is simulated by a new axially symmetric smooth potential of finite depth and width. The presence of additional potential parameters in this model allows us to describe the individual properties of different kinds of quantum dots. The influence of the Rashba and Dresselhaus spin-orbit interactions on electron states in quantum dot is investigated. The total Hamiltonian of the problem is written as a sum of unperturbed part and perturbation. First, the exact solution of the unperturbed Schrödinger equation was constructed. Each energy level of the unperturbed Hamiltonian was doubly degenerated. Further, the analytical approximate expression for energy splitting was obtained within the framework of perturbation theory, when the strengths of two spin-orbit interactions are close. The numerical results show the dependence of energy levels on potential parameters.

Keywords: circular quantum dots, confinement potential, spin-orbit interactions, energy levels.

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Introduction

The motion of an electron in an inner layer of a double semiconductor heterostructure is usually treated as two-dimensional in the (x, y) plane. In addition, the planar motion is also restricted if an electron is placed in a quantum dot localized in the middle layer of heterostructure. The Rashba V_R [1] and Dresselhaus V_D [2] interactions are presented by the formulas

$$V_R = \alpha_R(\sigma_x p_y - \sigma_y p_x)/\hbar, \quad V_D = \alpha_D(\sigma_x p_x - \sigma_y p_y)/\hbar, \tag{1}$$

where σ_x and σ_y are the standard Pauli spin-matrices. The strengths of these interactions depend on the materials used. The contributions of two spin-orbit interactions can be measured within various experimental methods [3, 4]. In the general case the whole spin-orbit interaction has the form $V_R + V_D$. At the same time, considerable attention is paid to the special case [3, 5, 6], when the spin-orbit interactions of Rashba and Dresselhaus have equal strength $\alpha_R = \alpha_D$. It can be experimentally achieved due to the fact that the Rashba interaction strength can be controlled by an external electric field, and the Dresselhaus interaction strength can be varied by changing the width of quantum well along the z axis [3, 7].

As a rule, circular quantum dots are simulated with the help of axially symmetric confinement potentials $V(x,y)=V(\rho)$, where $\rho=\sqrt{x^2+y^2}$. In [8, 9], a simple but sufficiently adequate rectangular potential of finite depth was proposed. This model with a discontinuous potential describes the main properties of circular quantum dots but without taking into account the individual characteristics. In [10], the smooth confinement potential of a new type which has finite depth and width was applied in the case of equal strengths $\alpha_R=\alpha_D$. The presence of additional potential parameters allows us to simulate different kinds of circular quantum dots. In the actual paper, we use this potential in order to calculate the energy levels of electron for unequal but close strengths $\alpha_R\neq\alpha_D$.

Methods and results

The circular quantum dot of radius ρ_0 is described by means of the confinement potential $V(\rho)=V_0 v(r)$, where V_0 is the depth of the potential well. The function $v(r)$ depends on ratio $r=\rho/\rho_0$ in the following way

$$v(r)=\begin{cases}0, & 0<r<g,\\ v_1(r), & g<r<s,\\ v_2(r), & s<r<1,\\ 1, & r>1.\end{cases} \tag{2}$$

The functions $v_1(r)$ and $v_2(r)$ have the following forms:

$$v_1(r)=d_1\left(r-\frac{g^2}{r}\right)^2,\quad d_1=\frac{1}{2}\frac{(1+s^2)}{(1-g^2)(s^2-g^2)}, \tag{3}$$

$$v_2(r)=1-d_2\left(r-\frac{1}{r}\right)^2,\quad d_2=\frac{1}{2}\frac{(g^2+s^2)}{(1-g^2)(1-s^2)}. \tag{4}$$

The parameters g and s change within ranges $0<g<1$ and $g<s<1$. The function $v(r)$ and its first derivative are continuous in the inflection points $r=g$, $r=s$ and $r=1$.

The total Hamiltonian of the problem can be written as a sum $H=H_0+H_1$, where

$$H_0=\frac{p_x^2+p_y^2}{2M_{eff}}+\frac{(\alpha_R+\alpha_D)}{2\hbar}(\sigma_x-\sigma_y)(p_x+p_y)+V(\rho), \tag{5}$$

$$H_1=\gamma\frac{(\alpha_R+\alpha_D)}{2\hbar}(\sigma_x+\sigma_y)(p_y-p_x),\quad \gamma=\frac{\alpha_R-\alpha_D}{\alpha_R+\alpha_D}, \tag{6}$$

M_{eff} is the effective electron mass which characterizes the motion in a semiconductor.

We shall solve the full Schrödinger equation $H\Psi=E\Psi$ in two stages. First, we obtain an exact solution of the unperturbed Schrödinger equation $H_0\Psi_0=E_0\Psi_0$ and then we shall take into account the perturbation H_1 within the framework of the perturbation theory.

By analogy with [10] it is easy to show that the required solutions of the unperturbed Schrödinger equation admit a factorization

$$\Psi_0^{\pm}(x,y)=\frac{1}{\sqrt{2}}\begin{pmatrix}1\\ \pm e^{-i\pi/4}\end{pmatrix}\exp\left(\mp i\frac{(\alpha_R+\alpha_D)M_{eff}(x+y)}{\sqrt{2}\hbar^2}\right)e^{im\phi}w(\rho), \tag{7}$$

where $m=0,\pm1,\pm2,\ldots$ is the angular momentum quantum number. Here we use the polar coordinates ρ,ϕ ($x=\rho\cos\phi, y=\rho\sin\phi$).

Introducing dimensionless quantities

$$e_0 = \frac{2M_{eff}\rho_0^2}{\hbar^2}E_0, \quad v_0 = \frac{2M_{eff}\rho_0^2}{\hbar^2}V_0, \quad a = \frac{M_{eff}\rho_0}{\hbar^2}(\alpha_R + \alpha_D), \tag{8}$$

we get the radial equation

$$\frac{d^2w}{dr^2} + \frac{1}{r}\frac{dw}{dr} - \frac{m^2w}{r^2} + \left(e_0 + a^2 - v_0 v(r)\right)w = 0. \tag{9}$$

It is seen that the wave function depends only on the combination $e_0 + a^2$.

In the region $0 < r < g$, the finite at $r \to 0$ solution of radial equation is expressed via the Bessel function [11] by means of the formula $w_1(r) = J_m\left(\sqrt{e_0 + a^2}\, r\right)$.

In the region $g < r < s$, it is simple to obtain two solutions in terms of the confluent hypergeometric functions [11]:

$$w_2(r) = r^B \exp\left(-\frac{\sqrt{d_1 v_0}}{2}r^2\right) M\left(A, 1+B, \sqrt{d_1 v_0}\, r^2\right), \tag{10}$$

$$w_3(r) = r^B \exp\left(-\frac{\sqrt{d_1 v_0}}{2}r^2\right) U\left(A, 1+B, \sqrt{d_1 v_0}\, r^2\right), \tag{11}$$

where

$$A = \frac{1+B}{2} - \frac{e_0 + a^2 + 2d_1 g^2 v_0}{4\sqrt{d_1 v_0}}, \quad B = \sqrt{m^2 + d_1 g^4 v_0}. \tag{12}$$

In the region $s < r < 1$, it is easy to show that two solutions are

$$w_4(r) = \frac{w_+(r) + w_-(r)}{2}, \quad w_5(r) = \frac{w_+(r) - w_-(r)}{2i}, \tag{13}$$

$$w_\pm(r) = r^{B_\pm} \exp\left(\mp\frac{\sqrt{-d_2 v_0}}{2}r^2\right) M\left(A_\pm, 1+B_\pm, \pm\sqrt{-d_2 v_0}\, r^2\right), \tag{14}$$

where

$$A_\pm = \frac{1+B_\pm}{2} \pm \frac{v_0 - e_0 - a^2 + 2d_2 v_0}{4\sqrt{-d_2 v_0}}, \quad B_\pm = \pm\sqrt{m^2 - d_2 v_0}. \tag{15}$$

Note that the functions $w_4(r)$ and $w_5(r)$ are real if $d_2 v_0 > m^2$.

In the region $r > 1$, the decreasing solution is expressed via the modified Bessel function [11] with the help of the formula $w_6(r) = K_m\left(\sqrt{v_0 - e_0 - a^2}\, r\right)$.

Thus, we obtain the radial wave function

$$w(r) = \begin{cases} c_1 w_1(r), & 0 < r < g, \\ c_2 w_2(r) + c_3 w_3(r), & g < r < s, \\ c_4 w_4(r) + c_5 w_5(r), & s < r < 1, \\ c_6 w_6(r), & r > 1. \end{cases} \tag{16}$$

The coefficients c_i are found from the continuity condition for function $w(r)$ and its first derivative $w'(r)$ at three inflection points $r = g$, $r = s$, and $r = 1$. The fulfilment of this condition and the continuity of the potential and its first derivative guarantee the continuity of the second and the third derivative of the wave function.

Six coefficients c_i satisfy six linear algebraic equations

$$T(g,s,v_0,m,a,e_0)\boldsymbol{X}=0, \tag{17}$$

where $\boldsymbol{X}=\{c_1,c_2,c_3,c_4,c_5,c_6\}$ and matrix T has the form

$$T(g,s,v_0,m,a,e_0)=\begin{pmatrix} w_1(g) & -w_2(g) & -w_3(g) & 0 & 0 & 0 \\ w_1'(g) & -w_2'(g) & -w_3'(g) & 0 & 0 & 0 \\ 0 & -w_2(s) & -w_3(s) & w_4(s) & w_5(s) & 0 \\ 0 & -w_2'(s) & -w_3'(s) & w_4'(s) & w_5'(s) & 0 \\ 0 & 0 & 0 & w_4(1) & w_5(1) & -w_6(1) \\ 0 & 0 & 0 & w_4'(1) & w_5'(1) & -w_6'(1) \end{pmatrix}. \tag{18}$$

Then the dependence of dimensionless energy $e_0(g,s,v_0,m,a)$ on three dimensionless potential parameters g, s, and v_0 is determined by the transcendental equation

$$k(g,s,v_0,m,a,e_0)=\det T(g,s,v_0,m,a,e_0)=0. \tag{19}$$

This equation is solved numerically. Each level of energy is degenerate with two eigenfunctions $\Psi_0^+(x,y)$ and $\Psi_0^-(x,y)$.

When the exact values of $e_0(g,s,v_0,m,a)$ are found it is not hard to obtain the values of coefficients c_i from the system (17) and the standard normalization condition.

So, the exact solution of the unperturbed Schrödinger equation is constructed for an electron in a circular quantum dot which is simulated by the smooth potential (2).

We introduce the dimensionless perturbation $h_1=2M_{eff}\rho_0^2H_1/\hbar^2$ and consider the contribution of h_1 with the help of the perturbation theory in the degenerate case for the small value of γ.

In the basis of the eigenvectors $|\Psi_0^+\rangle$ and $|\Psi_0^-\rangle$ of the unperturbed Hamiltonian we have the following equalities $\langle\Psi_0^\pm|h_1|\Psi_0^\pm\rangle=0$ for the diagonal matrix elements. Off-diagonal matrix elements are given by $\langle\Psi_0^+|h_1|\Psi_0^-\rangle=\langle\Psi_0^-|h_1|\Psi_0^+\rangle=\gamma\delta(m,v,a),$ where

$$\delta=-2ma\int_0^\infty J_1(2ar)w^2(r)dr\Big/\int_0^\infty w^2(r)r\,dr. \tag{20}$$

Then we get splitting $e^\pm=e_0\pm\gamma\delta$ for the energy levels. Normalized eigenfunctions in zero-order approximation, which correspond to the eigenvalues $e^\pm$, are described by the formula $\Psi^\pm=\left(\Psi_0^+\pm\Psi_0^-\right)/\sqrt{2}$. The distinctive feature of the used approximation is zero correction for zero angular momentum ($m=0$).

Now we present some numerical illustrations in addition to the analytical results. If we choose the value of effective electron mass $M_{eff}=0.067M_e$ related to GaAs, where M_e is the electron mass in vacuo, and assume $\rho_0=30$ nm, then the following correspondences $a=1\to(\alpha_R+\alpha_D)/2=18.9579$ meV nm, $e=1\to E=0.631933$ meV between the dimensionless and dimensional quantities are obtained.

Tab. 1, 2 demonstrate the dependence of energy levels on potential parameters at the following angular quantum numbers $m=0,\pm1,\pm2$. First of all we emphasize that the number of discrete levels is finite. This number increases if the parameters v_0 and g grow and decreases if m grows. The energy level decreases if the parameter s grows. The ratio δ/e_0 decreases if e_0 grows.

Table 1. The dependence of e_0 and δ on potential parameters for $a = 1$ and $v_0 = 100$

$\lvert m \rvert$	e_0, (δ)			
	$g = 0.1$		$g = 0.9$	
	$s = 0.325$	$s = 0.775$	$s = 0.925$	$s = 0.975$
0	37.8202 (0.00000)	21.1503 (0.00000)	4.36674 (0.00000)	4.20242 (0.00000)
	98.3459 (0.00000)	66.4228 (0.00000)	27.0087 (0.00000)	26.158 (0.00000)
	–	–	66.1516 (0.00000)	64.1934 (0.00000)
1	78.2272 (1.87550)	43.1724 (1.83448)	12.5861 (1.66374)	12.1710 (1.65410)
	–	87.9681 (1.61613)	43.8652 (1.65402)	42.5166 (1.64521)
	–	–	89.2195 (1.54573)	86.8404 (1.55437)
2	–	66.3115 (3.50209)	23.3249 (3.17680)	22.5838 (3.15368)
	–	–	62.8864 (3.22045)	61.0017 (3.20327)

Table 2. The dependence of e_0 and δ on potential parameters for $a = 1$ and $v_0 = 400$

$\lvert m \rvert$	e_0, (δ)			
	$g = 0.1$		$g = 0.9$	
	$s = 0.325$	$s = 0.775$	$s = 0.925$	$s = 0.975$
0	68.4065 (0.00000)	37.9282 (0.00000)	4.97095 (0.00000)	4.78748 (0.00000)
	248.296 (0.00000)	130.485 (0.00000)	30.4112 (0.00000)	29.4418 (0.00000)
	374.034 (0.00000)	223.558 (0.00000)	75.9617 (0.00000)	73.569 (0.00000)
	–	315.804 (0.00000)	141.174 (0.00000)	136.714 (0.00000)
	–	394.955 (0.00000)	225.085 (0.00000)	217.952 (0.00000)
	–	–	325.146 (0.00000)	315.041 (0.00000)
1	154.175 (1.95605)	82.8206 (1.91536)	14.1512 (1.69837)	13.6850 (1.68944)
	324.261 (1.87921)	176.327 (1.83530)	49.6767 (1.70195)	48.1080 (1.69318)
	398.235 (1.16738)	269.601 (1.75627)	105.147 (1.69960)	101.834 (1.69064)
	–	359.397 (1.64424)	179.906 (1.69342)	174.211 (1.68430)
	–	–	272.482 (1.67878)	263.873 (1.67029)
	–	–	377.369 (1.59580)	366.451 (1.61028)
2	244.117 (3.86453)	129.076 (3.74964)	26.2025 (3.26501)	25.3643 (3.24341)
	380.222 (3.53219)	222.626 (3.59204)	71.8550 (3.35158)	69.5931 (3.33240)
	–	315.315 (3.42475)	137.158 (3.36809)	132.829 (3.34919)
	–	396.324 (2.76619)	221.216 (3.36065)	214.206 (3.34202)
	–	–	321.637 (3.31530)	311.605 (3.30183)

Conclusion

The confinement model potential for a quantum dot considered in the present paper is smooth, has finite depth and width and permits the exact solutions of the separated unperturbed Schrödinger equation for electron states in the presence of the spin-orbit interaction of Rashba and Dresselhaus. The contribution of perturbation is really small in comparison with the unperturbed energy e_0 if the strength α_R is sufficiently close to the strength α_D ($\gamma \ll 1$). Further, we intend to construct higher-oder corrections to the energy levels.

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Authors' contribution

Both authors equally contributed to the writing of the article.

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