A.V. BARAN, V.V. KUDRYASHOV

Institute of Physics, National Academy of Sciences of Belarus
(68, Nezavisimosti Ave., Minsk 220072, Belarus; e-mail: a.baran@dragon.bas-net.by)

ENERGY LEVELS AND EIGENFUNCTIONS FOR TWO-DIMENSIONAL ELECTRON SYSTEMS WITH CONFINING SQUARE WELL POTENTIALS AND SPIN-ORBIT INTERACTIONS IN THE PRESENCE OF MAGNETIC FIELD

PACS 03.65Ge, 71.70.Ej, 73.21.-b

Solutions of the Schrödinger equation are obtained for electrons in two-dimensional circular semiconductor quantum dots and rings in the presence of both external uniform constant magnetic field and the Rashba and Dresselhaus spin-orbit interactions of equal strengths. Confinement is simulated by realistic square well potentials. The dependence of the energy levels on the magnetic field and the strength of spin-orbit interaction is presented in detail.

K e y w o r d s: circular quantum dots and rings, Rashba and Dresselhaus spin-orbit interactions, magnetic field.

1. Introduction

It is well known [1, 2] that the motion of an electron in an inner layer of a semiconductor heterostructure can be treated as two-dimensional in the (x, y) plane because of the existence of a confining quantum well along the z axis perpendicular to the (x, y) plane. In connection with the development of nanotechnology, the study of quantum dots and rings in heterostructures acquires the increasing importance. The confining potentials are usually assumed to be axially symmetric: $V_c(x, y) = V_c(\rho)$, where $\rho = \sqrt{x^2 + y^2}$. There are two types of confining potentials, which are widely employed in this area. First, the infinite hard walls are used to describe quantum dots [3, 4] and quantum rings [5, 6]. Second, the parabolic potentials are applied to simulate quantum dots [7, 8] and quantum rings [9, 10]. However, these models are unphysical in principle, because they do not permit the existence of unbound states in the absence of a magnetic field. The simple, but fairly adequate potentials of finite depth V were proposed in [11, 12] for the two-dimensional circular quantum dots and in [13, 14] for the quantum rings. These square well potentials are

$$V_c(\rho) = \begin{cases} 0, & 0 < \rho < \rho_o, \\ V, & \rho_o < \rho < \infty \end{cases} \tag{1}$$

in the case of quantum dots and

$$V_c(\rho) = \begin{cases} V, & 0 < \rho < \rho_i, \\ 0, & \rho_i < \rho < \rho_o, \\ V, & \rho_o < \rho < \infty \end{cases} \tag{2}$$

in the case of quantum rings. Here, ρ_o is the outer radius of a dot or ring, and ρ_i is the inner radius of a ring.

The influence of the Rashba [15, 16] and Dresselhaus [17] spin-orbit interactions on the electron states in planar heterostructures are widely studied in recent years. A uniform constant magnetic field B normal to the plane of quantum dots or rings is described by the vector potential $\mathbf{A} = \frac{B}{2}(-y, x, 0)$. Then the Rashba V_{R} and Dresselhaus V_{D} interactions are represented

by the formulas

$$V_{\rm R} = \alpha_{\rm R}(\sigma_x P_y - \sigma_y P_x)/\hbar,$$
$$V_{\rm D} = \alpha_{\rm D}(\sigma_x P_x - \sigma_y P_y)/\hbar, \tag{3}$$

where $\mathbf{P} = \mathbf{p} + q_e\mathbf{A}$, q_e is the absolute value of the electron charge, and σ_x and σ_y are the standard Pauli spin-matrices. The strengths of these interactions depend on the used materials. The contribution of two spin-orbit interactions can be measured within various experimental methods [2, 18].

The presence of an external magnetic field leads to the Zeeman interaction

$$H' = \tfrac{1}{2} g\mu_{\rm B} B\sigma_z, \tag{4}$$

where g is the effective gyromagnetic factor, $\mu_{\rm B} = \frac{q_e\hbar}{2M_e}$ is the Bohr magneton, M_e is the electron mass, and σ_z is the Pauli matrix. Thus, the total Hamiltonian of the problem can be written in the following way:

$$H_{\rm total} = \frac{P_x^2 + P_y^2}{2M_{\rm eff}} + V_c(\rho) + V_{\rm R} + V_{\rm D} + H', \tag{5}$$

where $M_{\rm eff}$ is the effective electron mass, and $V_c(\rho)$ is of the form (1) or (2). In the general case with arbitrary values of $\alpha_{\rm R}$ and $\alpha_{\rm D}$, the exact solutions of the Schrödinger equation with Hamiltonian (5) are unknown. In the particular case of the Rashba interaction ($\alpha_{\rm D} = 0$), the exact solutions were obtained in [19] for quantum dots and in [20] for quantum rings. Note that it is easy to find the similar exact solutions in the opposite particular case of the Dresselhaus interaction ($\alpha_{\rm R} = 0$).

At the same time, the considerable attention is paid to the special case [2, 21, 22] where the spin-orbit interactions of Rashba and Dresselhaus have equal strength $\alpha_{\rm R} = \alpha_{\rm D} = \alpha$, which 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 a quantum well along the z axis [1, 2]. In the present paper for the special case $\alpha_{\rm R} = \alpha_{\rm D}$, we obtain the wave functions, as well as the dependence of the energy levels on the magnetic field and the spin-orbit interaction strength. The calculations are performed for the parameter values associated with GaAs.

2. Exact Solution of the Unperturbed Schrödinger Equation without the Zeeman Interaction

In the considered case where $\alpha_{\rm R} = \alpha_{\rm D}$, the Hamiltonian can be represented as a sum

$$H = H_0 + H' \tag{6}$$

of the unperturbed part

$$H_0 = \frac{P_x^2 + P_y^2}{2M_{\rm eff}} + V_c(\rho) + \frac{\alpha}{\hbar}(\sigma_x - \sigma_y)(P_x + P_y) \tag{7}$$

and the perturbation described by the Zeeman interaction. It should be stressed that H_0 depends on the magnetic field, which is contained in the definition of P_x and P_y.

We solve the full Schrödinger equation $H\Psi = E\Psi$ in two stages. First, we will obtain an exact solution of the unperturbed Schrodinger equation

$$H_0\Psi_0 = E_0\Psi_0 \tag{8}$$

and then we take the Zeeman interaction into account within the framework of perturbation theory.

Let us consider the case of the unperturbed equation (8) with Hamiltonian (7). It is easy to see that, in addition to the obvious integral of motion

$$\sigma = (\sigma_x - \sigma_y)/\sqrt{2}, \tag{9}$$

there is also the non-trivial integral of motion

$$L = L_z + \alpha M_{\rm eff}(x - y)(\sigma_x - \sigma_y)/\hbar, \tag{10}$$

where L_z is the operator of angular momentum.

We look for the solutions of Eq. (8), which are eigenfunctions of the operators σ and L. Then the required solutions admit a factorization of the form

$$\Psi_0^{\pm}(x, y) = \mathbf{n}^{\pm} e^{\mp i\sqrt{2}\,\alpha M_{\rm eff}(x+y)/\hbar^2} e^{im\phi} u(\rho), \tag{11}$$

where m is the angular momentum quantum number ($m = 0, \pm1, \pm2, ...$), $\mathbf{n}^{\pm}$ are eigenvectors of the operator σ:

$$\sigma\,\mathbf{n}^{\pm} = \pm\mathbf{n}^{\pm}, \quad \mathbf{n}^{\pm} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ \pm e^{-i\pi/4} \end{pmatrix}. \tag{12}$$

Here, we use the polar coordinates ρ, ϕ ($x = \rho\cos\phi$, $y = \rho\sin\phi$).

The obtained wave functions satisfy the relations

$$\sigma\,\Psi_0^{\pm}(x,y) = \pm\Psi_0^{\pm}(x,y),$$
$$L\,\Psi_0^{\pm}(x,y) = m\hbar\,\Psi_0^{\pm}(x,y). \tag{13}$$

Introducing the dimensionless quantities

$$r = \frac{\rho}{\rho_o}, \quad e_0 = \frac{2M_{\rm eff}\rho_o^2}{\hbar^2}\,E_0, \quad v = \frac{2M_{\rm eff}\rho_o^2}{\hbar^2}\,V,$$
$$a = \frac{2M_{\rm eff}\rho_o}{\hbar^2}\,\alpha, \quad b = \frac{q_e\rho_o^2}{2\hbar}\,B, \tag{14}$$

we write the radial equation

$$\frac{d^2u}{d\,r^2} + \frac{1}{r}\frac{d\,u}{d\,r} - \left(\frac{m^2}{r^2} - 2bm - b^2r^2\right)u +$$
$$+\left(e_0 + a^2 - v_c(r)\right)u = 0, \tag{15}$$

where

$$v_c(r) = \begin{cases} 0, & 0 < r < 1, \\ v, & 1 < r < \infty \end{cases} \tag{16}$$

for the quantum dots and

$$v_c(r) = \begin{cases} v, & 0 < r < r_i, \\ 0, & r_i < r < 1, \\ v, & 1 < r < \infty \end{cases} \tag{17}$$

for the quantum rings. Here, we use the notation $r_i = \rho_i/\rho_o$ for the relative width of a ring.

Note that the equation considered in [23] for the radial wave function of an electron in a uniform magnetic field without taking the spin-orbit interaction into account coincides with Eq. (15) if the replacement $e_0 \to e_0 + a^2 - v_c(r)$ is performed in all regions defined in (16) and (17). Therefore, following [23], we represent a required function $u(r)$ by the formula

$$u(r) = \left(br^2\right)^{\frac{|m|}{2}} \exp\left(\frac{-br^2}{2}\right) w(r). \tag{18}$$

The function $w(r)$ is expressed in terms of the confluent hypergeometric functions of the first and second kinds $M(\gamma,\beta,\xi)$ and $U(\gamma,\beta,\xi)$ [24]. The particular solutions are chosen so that the radial wave functions are regular at the origin $r \to 0$ and tend to zero, as $r \to \infty$. We demand the fulfilment of continuity conditions for the function $w(r)$ and its first derivative $w'(r) = dw(r)/dr$ at the boundary points.

For the quantum dots, we derive the explicit formulas

$$w(r) = \begin{cases} \tilde{c}_1\tilde{w}_1(r), & 0 < r < 1, \\ \tilde{c}_2\tilde{w}_2(r), & 1 < r < \infty, \end{cases} \tag{19}$$

where

$$\tilde{w}_1(r) = M\left(\gamma_i,\beta,br^2\right), \quad \tilde{w}_2(r) = U\left(\gamma_o,\beta,br^2\right), \tag{20}$$

$$\gamma_o = \frac{m+|m|+1}{2} - \frac{e_0+a^2-v}{4b},$$
$$\gamma_i = \frac{m+|m|+1}{2} - \frac{e_0+a^2}{4b}, \quad \beta = |m|+1. \tag{21}$$

The continuity condition at the boundary point $r = 1$ leads to the system of algebraic equations

$$T_2(m,e_0,v,a,b)\tilde{\mathbf{X}} = 0 \tag{22}$$

for two coefficients, where $\tilde{\mathbf{X}} = \{\tilde{c}_1,\tilde{c}_2\}$, and $T_2(m,e_0,v,a,b)$ is a 2×2 matrix of the form

$$T_2 = \begin{pmatrix} \tilde{w}_1(1) & -\tilde{w}_2(1) \\ \tilde{w}_1'(1) & -\tilde{w}_2'(1) \end{pmatrix}. \tag{23}$$

Hence, the exact equation for $e_o(m,v,a,b)$ is

$$\det T_2 = \gamma_o M(\gamma_i,\beta,b)U(\gamma_o+1,\beta+1,b) +$$
$$+\frac{\gamma_i}{\beta}U(\gamma_o,\beta,b)M(\gamma_i+1,\beta+1,b) = 0. \tag{24}$$

The coefficients $\tilde{c}_1$ and $\tilde{c}_2$ are connected by relation

$$\tilde{c}_2 = \tilde{c}_1 M(\gamma_i,\beta,b)/U(\gamma_o,\beta,b), \tag{25}$$

and the value of $\tilde{c}_1$ is obtained from the normalization condition $\langle\Psi_0^{\pm}|\Psi_0^{\pm}\rangle = 1$.

For the quantum rings, we obtain the expressions

$$w(r) = \begin{cases} c_1w_1(r), & 0 < r < r_i, \\ c_{21}w_{21}(r) + c_{22}w_{22}(r), & r_i < r < 1, \\ c_3w_3(r), & 1 < r < \infty, \end{cases} \tag{26}$$

where

$$w_1(r) = M\left(\gamma_o,\beta,br^2\right), \quad w_{21}(r) = M\left(\gamma_i,\beta,br^2\right),$$
$$w_3(r) = U\left(\gamma_o,\beta,br^2\right), \quad w_{22}(r) = U\left(\gamma_i,\beta,br^2\right). \tag{27}$$

In this case, the continuity conditions at the boundary points $r = r_i$ and $r = 1$ lead to the system of algebraic equations

$$T_4(m,e_0,v,a,b,r_i)\mathbf{X} = 0 \tag{28}$$

for four coefficients, where $\mathbf{X} = \{c_1, c_{21}, c_{22}, c_3\}$, and $T_4(m, e_0, v, a, b, r_i)$ is a 4×4 matrix of the form

$$T_4 = \begin{pmatrix} w_1(r_i) & -w_{21}(r_i) & -w_{22}(r_i) & 0 \\ w_1'(r_i) & -w_{21}'(r_i) & -w_{22}'(r_i) & 0 \\ 0 & w_{21}(1) & w_{22}(1) & -w_3(1) \\ 0 & w_{21}'(1) & w_{22}'(1) & -w_3'(1) \end{pmatrix}. \quad (29)$$

Now, we determine $e_0(m, v, a, b, r_i)$ as a solution of the equation

$$\det T_4(m, e_0, v, a, b, r_i) = 0. \quad (30)$$

In order to construct the radial wave function completely, we find the values of required coefficients

$$\begin{pmatrix} c_{21} \\ c_{22} \\ c_3 \end{pmatrix} = -c_1 T_3^{-1}(m, e_0, v, a, b, r_i) \begin{pmatrix} w_1'(r_i) \\ 0 \\ 0 \end{pmatrix}, \quad (31)$$

where

$$T_3 = \begin{pmatrix} -w_{21}'(r_i) & -w_{22}'(r_i) & 0 \\ w_{21}(1) & w_{22}(1) & -w_3(1) \\ w_{21}'(1) & w_{22}'(1) & -w_3'(1) \end{pmatrix}. \quad (32)$$

The residual arbitrariness in the choice of the coefficient c_1 is used to implement the standard normalization condition.

We also use the notation $e_o(m, v, a, b, r_i)$ for the quantum dots keeping in mind that, in this case, $r_i = 0$. From Eq. (15), we see that the dependence of e_0 on a is trivial: $e_0(m, v, a, b, r_i) = e_o(m, v, 0, b, r_i) - a^2$. In addition, the relation $e_0(m, v, a, b, r_i) - e_0(-m, v, a, b, r_i) = 4bm$ is satisfied. Of course, Eqs. (24) and (30) cannot be solved analytically, but can be easily solved numerically.

3. Contribution of the Zeeman Interaction within the Framework of Perturbation Theory

The expression for the Zeeman interaction in dimensionless quantities takes the form

$$h' = \frac{2M_{\text{eff}}\rho_o^2}{\hbar^2} H' = 4sb\,\sigma_z, \quad s = \frac{gM_{\text{eff}}}{4M_e}. \quad (33)$$

Since each energy level of the unperturbed system is doubly degenerate with two eigenfunctions (11), we consider the contribution of the Zeeman interaction with the help of perturbation theory in the degenerate case.

Because of $\sigma_z\,\mathbf{n}^{\pm} = \mathbf{n}^{\mp}$, we have the equalities

$$\langle \Psi_0^{\pm} | \sigma_z | \Psi_0^{\pm} \rangle = 0 \quad (34)$$

for the diagonal matrix elements in the basis of the eigenvectors $|\Psi_0^+\rangle$ and $|\Psi_0^-\rangle$ of the unperturbed Hamiltonian. The off-diagonal matrix elements are given by

$$\langle \Psi_0^+ | \sigma_z | \Psi_0^- \rangle = \langle \Psi_0^- | \sigma_z | \Psi_0^+ \rangle = \delta(m, v, a, b, r_i), \quad (35)$$

where

$$\delta(m, v, a, b, r_i) = \frac{\int\limits_0^\infty J_0(2ar) u^2(r) r\,dr}{\int\limits_0^\infty u^2(r) r\,dr} \quad (36)$$

in terms of the Bessel function.

Then we get the splitting

$$e^{\pm} = e_0 \pm e' \quad (37)$$

for the unperturbed energy levels, where

$$e' \equiv e'(m, v, a, b, r_i) = 4sb\,\delta(m, v, a, b, r_i). \quad (38)$$

The relation $e'(-m, v, a, b, r_i) = e'(m, v, a, b, r_i)$ is fulfilled for the corrections e'. The normalized eigenfunctions in the zero-order approximation, which correspond to the eigenvalues $e^{\pm}$, are described by the formulas

$$\Psi^{\pm} = \frac{1}{\sqrt{2}} \left(\Psi_0^+ \pm \Psi_0^- \right). \quad (39)$$

Note that, in the limiting case $\alpha = 0$, expressions (37) and (39) become exact.

4. Numerical Results

Now, we present some graphic illustrations in addition to the analytical results. In accordance with [4], we choose the parameters $M_{\text{eff}} = 0.067 M_e$ and $g = -0.44$ related to GaAs. Then we get $s = -0.00737$.

If we assume $\rho_o = 30$ nm, then the following correspondences $a = 1 \to \alpha = 18.9579$ meV nm, $e = 1 \to E = 0.631933$ meV between the dimensionless and dimensional quantities are obtained. For example, at the chosen parameters, the dimensionless value $v = 400$ corresponds to the potential well depth $V = 252.772$ meV, which is close to the value 257 meV in [14].

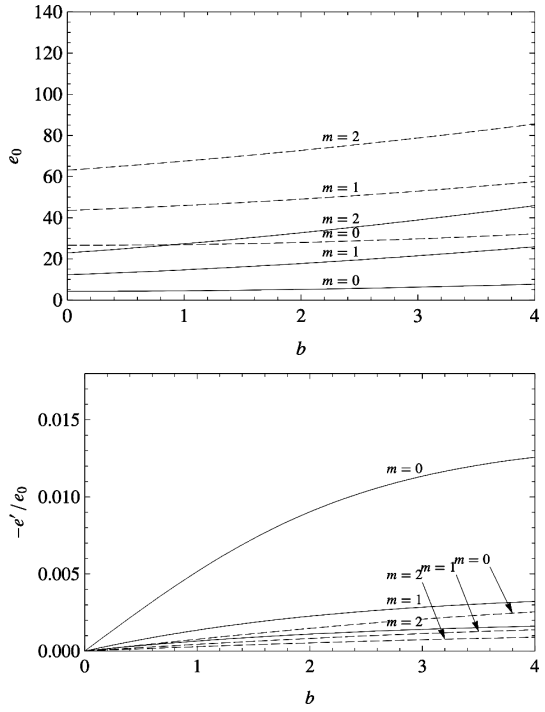

Fig. 1. Dependences of e_0 and $-e'/e_0$ on b at $a = 1$ for a quantum dot ($r_i = 0$)

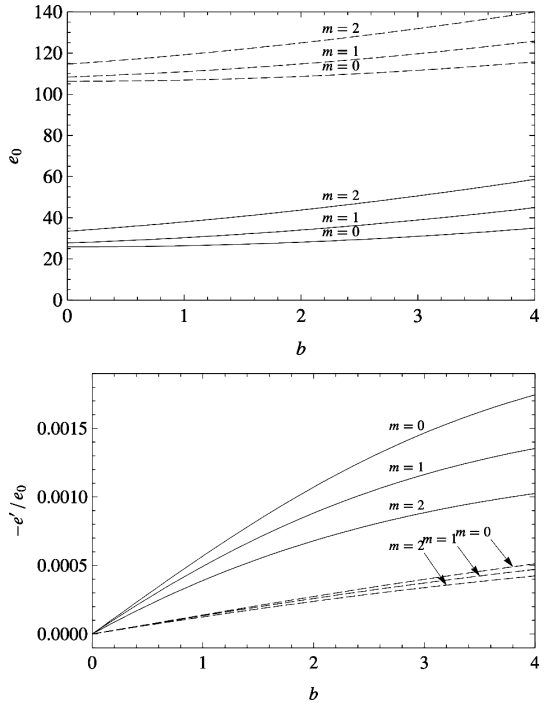

Fig. 2. Dependences of e_0 and $-e'/e_0$ on b at $a = 1$ for a quantum ring ($r_i = 0.5$)

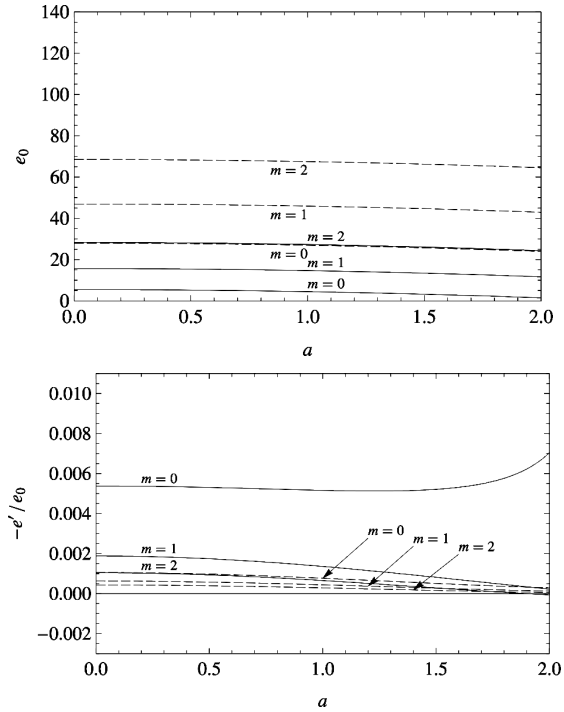

Fig. 3. Dependences of e_0 and $-e'/e_0$ on a at $b = 1$ for a quantum dot ($r_i = 0$)

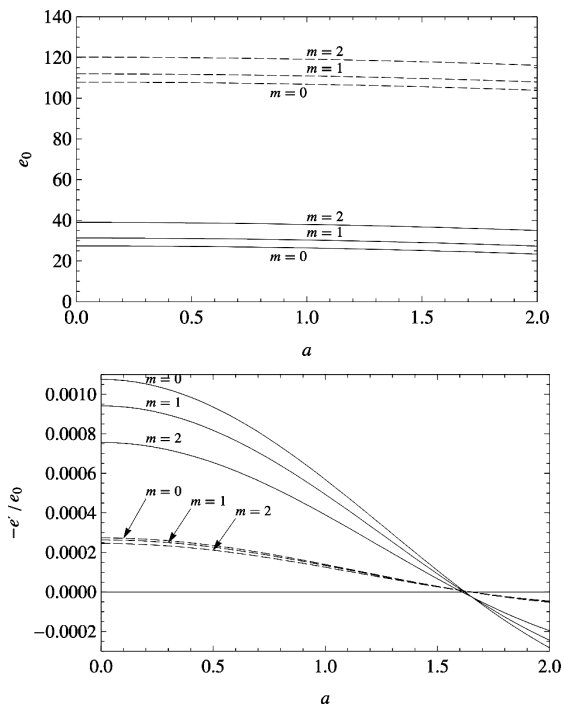

Fig. 4. Dependence of e_0 and $-e'/e_0$ on a at $b = 1$ for a quantum ring ($r_i = 0.5$)

Figures 1 and 2 show the dependences of the unperturbed energy e_0 and the relative correction $-e'/e_0$ to the energy on a magnetic field b in the dimensionless form at the fixed value of spin-orbit interaction strength a for the quantum dots ($r_i = 0$) and the quantum rings ($r_i = 0.5$).

Figures 3 and 4 demonstrate the dependences of e_0 and $-e'/e_0$ on a at a fixed value of b. The solid lines represent the first energy levels, and the dashed lines represent the second levels for three values of angular momentum ($m = 0, 1, 2$).

In connection with Figs. 3 and 4, it should be noted that the relative corrections $-e'/e_0$ are equal to zero at $a = 1.897$ for the quantum dots and at $a = 1.609,\ 1.619,\ 1.623,\ 1.647,\ 1.648,\ 1.649$ for the quantum rings. Of course, this circumstance does not indicate the disappearance of the Zeeman interaction, but demonstrates a property of the lower approximation. The contribution of the Zeeman interaction will appear in higher approximations for all values of parameter a.

5. Conclusion

The wave functions and the energy levels are obtained for electrons in two-dimensional quantum dots and rings with regard for the Rashba and Dresselhaus spin-orbit interactions of equal strengths in the presence of an external uniform constant magnetic field in the framework of an adequate model with a finite-depth confining potential. These results may be of interest in the study of spin-dependent effects in semiconductor heterostructures.

1. M. Valín-Rodríguez, A. Puente, and L. Serra, Eur. Phys. J. B **39**, 87 (2004).
2. J. Li and K. Chang, Phys. Rev. B **82**, 033304 (2010).
3. E.N. Bulgakov and A.F. Sadreev, JETP Lett. **73**, 505 (2001).
4. E. Tsitsishvili, G.S. Lozano, and A.O. Gogolin, Phys. Rev. B **70**, 115316 (2004).
5. J.S. Sheng and Kai Chang, Phys. Rev. B **74**, 235315 (2006).
6. J. Song and S.E. Ulloa, Phys. Rev. B **63**, 125302 (2001).
7. Rogerio de Sousa and S. Das Sarma, Phys. Rev. B **68**, 153330 (2003).
8. W.H. Kuan, S.C. Tang, and W. Xu, J. Appl. Phys. **95**, 6368 (2004).
9. M. Valín-Rodríguez, A. Puente, and L. Serra, Eur. Phys. J. D **12**, 493 (2000).
10. A.O. Govorov, S.E. Ulloa, K. Karrai, and R.J. Warburton, Phys. Rev. B **66**, 081309 (2002).
11. V.V. Kudryashov, Proc. of the XIII Intern. School-Conference "Foundations and Advances in Nonlinear Science", Minsk (2006), p. 125.
12. A.V. Chaplik and L.I. Magarill, Phys. Rev. Lett. **96**, 126402 (2006).
13. T.V. Bandos, A. Cantarero, and A. Garcia-Cristóbal, Eur. Phys. J. B **53**, 99 (2006).
14. M. Grochol, F. Grosse, and R. Zimmermann, Phys. Rev. B **74**, 115416 (2006).
15. E.I. Rashba, Sov. Phys. Solid State **2**, 1224 (1960).
16. Yu.A. Bychkov and E.I. Rashba, J. Phys. C **17**, 6039 (1984).
17. G. Dresselhaus, Phys. Rev. **100**, 580 (1955).
18. L. Meier *et al.*, Nature Phys. **3**, 650 (2007).
19. V.V. Kudryashov, Proceedings of the Fourteenth Annual Seminar "NPCS 2007", Minsk (2007), p. 75.
20. V.V. Kudryashov and A.V. Baran, Nonlin. Phenom. Complex Syst. **14**, 89 (2011).
21. J. Schliemann, J.C. Egues, and D. Loss, Phys. Rev. Lett. **90**, 14680 (2003).
22. B.A. Bernevig, J. Orenstein, and S.C. Zhang, Phys. Rev. Lett. **97**, 236601 (2006).
23. L.D. Landau and E.M. Lifshitz, *Quantum Mechanics, Nonrelativistic Theory* (Pergamon Press, Oxford, 1977).
24. M. Abramovitz and I.A. Stegun, *Handbook of Mathematical Functions* (Dover, New York, 1970).

Received 28.02.14

А.В. Баран, В.В. Кудряшов

РІВНІ ЕНЕРГІЇ І ВЛАСНІ ФУНКЦІЇ ДВОВИМІРНИХ ЕЛЕКТРОННИХ СИСТЕМ З УТРИМУЮЧИМИ ПРЯМОКУТНИМИ ПОТЕНЦІАЛАМИ І СПІН-ОРБІТАЛЬНИМИ ВЗАЄМОДІЯМИ У ПРИСУТНОСТІ МАГНІТНОГО ПОЛЯ

Р е з ю м е

Отримано рішення рівняння Шредінгера для електронів у двовимірних кругових напівпровідникових квантових точках і кільцях у присутності зовнішнього постійного однорідного магнітного поля та спін-орбітальних взаємодій Рашби і Дрессельхауса рівних інтенсивностей. Конфайнмент моделюється реалістичними прямокутними потенціалами. Представлено залежність рівнів енергії від магнітного поля та інтенсивності спін-орбітальної взаємодії.