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Rashba coupling in quantum dots in the presence of magnetic field

V.V. Kudryashov*
Institute of Physics, National Academy of Sciences of Belarus
68 Nezavisimosti Ave., 220072, Minsk, Belarus

We present an analytical solution to the Schrodinger equation for electron in a two-dimensional circular quantum dot in the presence of both external magnetic field and the Rashba spin-orbit interaction. The confinement is described by the realistic potential well of finite depth.

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1. Introduction

The Schrödinger equation describing electron in a two-dimensional quantum dot normal to the z axis is of the form

$$\left(\frac{\mathbf{P}^2}{2M_{eff}} + V_c(x,y) + V_R + V_Z\right)\Psi = E\Psi \tag{1}$$

where M_{eff} is the effective electron mass. The vector potential $\mathbf{A} = \frac{B}{2}(-y, x, 0)$ of a magnetic field oriented perpendicular to the plane of the quantum dot leads to the generalized momentum $\mathbf{P} = \mathbf{p} + \frac{e}{c}\mathbf{A}$. We have the usual expression for the Zeeman interaction

$$V_Z = \frac{1}{2} g\mu_B B\sigma_z \tag{2}$$

where g represents the effective gyromagnetic factor, μ_B is the Bohr's magneton The Rashba spin-orbit interaction [1, 2] is represented as

$$V_R = a_R(\sigma_x P_y - \sigma_y P_x). \tag{3}$$

The Pauli spin-matrices are defined as standard.

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

A confining potential is usually assumed to be symmetric,$V_c(x,y) = V_c(\rho), \rho = \sqrt{x^2+y^2}$. There are two model potentials which are widely employed in this area. The first is a harmonic oscillator potential [3, 4]. Such a model admits the approximate (not exact) solutions of Eq. (1). The second model is a circular quantum dot with hard walls [5, 6] $V_c(\rho) = 0$ for $\rho < \rho_0$, $V_c(\rho) = \infty$ for $\rho > \rho_0$. This model is exactly solvable. In the framework of above models the number of allowed energy levels is infinite for the fixed total angular momentum in the absence of a magnetic field.

*E-mail: kudryash@dragon.bas-net.by

In this paper, we propose new model which corresponds to a circular quantum dot with a potential well of finite depth: $V_c(\rho) = 0$ for $\rho < \rho_0$, $V_c(\rho) = V = constant$ for $\rho > \rho_0$. Our model is exactly solvable and the number of admissible energy levels is finite for the fixed total angular momentum in the absence of a magnetic field. The present solutions contain, as limiting cases, our previous results [7] (no external magnetic field).

2. Analytical solutions of the Schrödinger equation

The Schrödinger equation (1) is considered in the cylindrical coordinates $x = \rho\cos\varphi, y = \rho\sin\varphi$. Further it is convenient to employ dimensionless quantities

$$r = \frac{\rho}{\rho_0}, \quad \epsilon = \frac{2M_{eff}}{\hbar^2}\rho_0^2 E, \quad v = \frac{2M_{eff}}{\hbar^2}\rho_0^2 V, \quad a = \frac{2M_{eff}}{\hbar}\rho_0 a_R, \quad b = \frac{eB\rho_0^2}{2c\hbar}, \quad s = \frac{gM_{eff}}{4M_e}. \tag{4}$$

Here M_e is the electron mass. As it was shown in [5] equation (1) permits the separation of variables

$$\Psi_m(r,\varphi) = u(r)e^{im\varphi}\begin{pmatrix}1\\0\end{pmatrix} + w(r)e^{i(m+1)\varphi}\begin{pmatrix}0\\1\end{pmatrix}, \quad m = 0, \pm1, \pm2, \ldots \tag{5}$$

due to conservation of the total angular momentum $L_z + \frac{\hbar}{2}\sigma_z$.

We have the following radial equations

$$\begin{aligned}
&\frac{d^2u}{dr^2} + \frac{1}{r}\frac{du}{dr} + (\epsilon - v)u - \frac{m^2}{r^2}u - 2bmu - b^2r^2u - 4sbu \\
&\qquad = a\left(\frac{dw}{dr} + \frac{m+1}{r}w + brw\right) = 0, \\
&\frac{d^2w}{dr^2} + \frac{1}{r}\frac{dw}{dr} + (\epsilon - v)w - \frac{(m+1)^2}{r^2}w - 2b(m+1)w - b^2r^2w + 4sbw \\
&\qquad = a\left(-\frac{du}{dr} + \frac{m}{r}u + bru\right) = 0.
\end{aligned} \tag{6}$$

In [5, 6], the requirements $u(1) = w(1) = 0$ were imposed. In our model, we look for the radial wave functions $u(r)$ and $w(r)$ regular at the origin $r = 0$ and decreasing at infinity $r \to \infty$.

Following [6] we use the substitutions

$$u(r) = \exp\left(\frac{-br^2}{2}\right) r^{|m|} f(br^2), \quad w(r) = \exp\left(\frac{-br^2}{2}\right) r^{|m+1|} g(br^2) \tag{7}$$

which lead to the confluent hypergeometric equations in the case $a = 0$. Therefore we attempt to express the desired solutions of Eq. (6) via the confluent hypergeometric functions when $a \neq 0$.

We consider two regions $r < 1$ (region 1) and $r > 1$ (region 2) separately.

In the region 1 ($v = 0$), using the known properties

$$\begin{aligned}
M(\alpha,\beta,\xi) - \frac{dM(\alpha,\beta,\xi)}{d\xi} &= \frac{\beta-\alpha}{\beta}M(\alpha,\beta+1,\xi), \\
(\beta - 1 - \xi)M(\alpha,\beta,\xi) + \xi\frac{dM(\alpha,\beta,\xi)}{d\xi} &= (\beta-1)M(\alpha-1,\beta-1,\xi)
\end{aligned} \tag{8}$$

of the confluent hypergeometric functions $M(\alpha, \beta, \xi)$ of the first kind [8] it is easily to show that the suitable particular solutions of the radial equations are

$$u_1(r) = \exp\left(\frac{-br^2}{2}\right) r^{|m|} \left(c_{1-} f_{1-}(r) + c_{1+} f_{1+}(r)\right),$$
$$w_1(r) = \exp\left(\frac{-br^2}{2}\right) r^{|m+1|} \left(\frac{a}{2\sqrt{b}}\right) \left(c_{1-} g_{1-}(r) + c_{1+} g_{1+}(r)\right), \tag{9}$$

where

$$f_{1\mp}(r) = M(m+1-k_1^{\mp}, m+1, br^2),$$
$$g_{1\mp}(r) = \left(\frac{k_1^{\mp}}{(m+1)}\right) \frac{M(m+1-k_1^{\mp}, m+2, br^2)}{(-k_1^{\mp} + (4b)^{-1}\epsilon + s - 1/2)} \tag{10}$$

for $m = 0, 1, 2...$,

$$f_{1\mp}(r) = M(1-k_1^{\mp}, -m+1, br^2),$$
$$g_{1\mp}(r) = m \frac{M(-k_1^{\mp}, -m+, br^2)}{(-k_1^{\mp} + (4b)^{-1}\epsilon + s - 1/2)} \tag{11}$$

for $m = -1, -2, -3...$ and

$$k_1^{\pm} = \frac{1}{4b}\left(\epsilon + \frac{a^2}{2} \pm a\sqrt{\epsilon + \frac{a^2}{4} + \left(\frac{4b}{a}\right)^2 (s-1/2)^2}\right). \tag{12}$$

Here c_{1-} and c_{1+} are arbitrary coefficients. The functions $u_1(r)$ and $w_1(r)$ have the desirable behavior at the origin.

In the region 2 ($v > 0$), using the known properties

$$U(\alpha, \beta, \xi) - \frac{dU(\alpha, \beta, \xi)}{d\xi} = U(\alpha, \beta+1, \xi),$$
$$(\beta - 1 - \xi)U(\alpha, \beta, \xi) + \xi\frac{dU(\alpha, \beta, \xi)}{d\xi} = -U(\alpha-1, \beta-1, \xi) \tag{13}$$

of the confluent hypergeometric functions $U(\alpha, \beta, \xi)$ of the second kind [8] it is simply to get the suitable real solutions of the radial equations:

$$u_2(r) = \exp\left(\frac{-br^2}{2}\right) r^{|m|} \left(c_{2-} f_{2-}(r) + c_{2+} f_{2+}(r)\right),$$
$$w_2(r) = \exp\left(\frac{-br^2}{2}\right) r^{|m+1|} \left(\frac{a}{2\sqrt{b}}\right) \left(c_{2-} g_{2-}(r) + c_{2+} g_{2+}(r)\right), \tag{14}$$

where

$$f_{2\mp}(r) = \frac{\sqrt{\mp 1}}{2}\left(U(m+1-k_2^-, m+1, br^2) \mp U(m+1-k_2^+, m+1, br^2)\right),$$
$$g_{2\mp}(r) = \frac{\sqrt{\mp 1}}{2}\left(\frac{U(m+1-k_2^-, m+2, br^2)}{(-k_2^- + (4b)^{-1}(\epsilon - v) + s - 1/2)} \mp \frac{U(m+1-k_2^+, m+2, br^2)}{(-k_2^+ + (4b)^{-1}(\epsilon - v) + s - 1/2)}\right) \tag{15}$$

for $m = 0, 1, 2...$,

$$f_{2\mp}(r) = \frac{\sqrt{\mp 1}}{2}\left(U(1-k_2^-, -m+1, br^2) \mp U(1-k_2^+, -m+1, br^2)\right),$$
$$g_{2\mp}(r) = \frac{\sqrt{\mp 1}}{2}\left(\frac{U(-k_2^-, -m, br^2)}{(-k_2^- + (4b)^{-1}(\epsilon - v) + s - 1/2)} \mp \frac{U(-k_2^+, -m, br^2)}{(-k_2^+ + (4b)^{-1}(\epsilon - v) + s - 1/2)}\right) \tag{16}$$

for $m = -1, -2, -3...$ and

$$k_2^{\pm} = \frac{1}{4b}\left(\epsilon - v + \frac{a^2}{2} \pm ia\sqrt{v - \epsilon - \frac{a^2}{4} - \left(\frac{4b}{a}\right)^2 (s-1/2)^2}\right). \tag{17}$$

Here c_{2-} and c_{2+} are arbitrary coefficients. The functions $u_2(r)$ and $w_2(r)$ have the appropriate behavior at infinity.

We assume the realization of condition

$$\epsilon < v^* = v - \frac{a^2}{4} - \left(\frac{4b}{a}\right)^2 (s-1/2)^2 \tag{18}$$

which means that electron belongs to a quantum dot. We can also obtain the exact solutions when $\epsilon > v^*$. However, in this case we cannot consider electron as belonging to a quantum dot.

The continuity conditions

$$u_1(1) - u_2(1) = 0, \quad w_1(1) - w_2(1) = 0, \quad u_1'(1) - u_2'(1) = 0, \quad w_1'(1) - w_2'(1) = 0 \tag{19}$$

for the radial wave functions and their derivatives at the boundary point $r = 1$ lead to the algebraic equations

$$T_4(m, \epsilon, v.a, b, s)\begin{pmatrix} c_{1-} \\ c_{1+} \\ c_{2-} \\ c_{2+} \end{pmatrix} = 0 \tag{20}$$

for coefficients c_{1-}, c_{1+}, c_{2-} and c_{2+} where

$$T_4(m, \epsilon, v.a, b, s) = \begin{pmatrix} f_{1-}(1) & f_{1+}(1) & -f_{2-}(1) & -f_{2+}(1) \\ g_{1-}(1) & g_{1+}(1) & -g_{2-}(1) & -g_{2+}(1) \\ f_{1-}'(1) & f_{1+}'(1) & -f_{2-}'(1) & -f_{2+}'(1) \\ g_{1-}'(1) & g_{1+}'(1) & -g_{2-}'(1) & -g_{2+}'(1) \end{pmatrix}. \tag{21}$$

Hence, the exact equation for energy $\epsilon(m, v, a, b, s)$ is

$$\det T_4(m, \epsilon, v, a, b, s) = 0. \tag{22}$$

This equation is solved numerically.

The desired coefficients are

$$\begin{pmatrix} c_{1+} \\ c_{2-} \\ c_{2+} \end{pmatrix} = c_{1-} T_3^{-1}(m, \epsilon, v, a, b, s)\begin{pmatrix} -f_{1-}(1) \\ -g_{1-}(1) \\ -f_{1-}'(1) \end{pmatrix} \tag{23}$$

where

$$T_3(m, \epsilon, v, a, b, s) = \begin{pmatrix} f_{1+}(1) & -f_{2-}(1) & -f_{2+}(1) \\ g_{1+}(1) & -g_{2-}(1) & -g_{2+}(1) \\ f_{1+}'(1) & -f_{2-}'(1) & -f_{2+}'(1) \end{pmatrix}. \tag{24}$$

The value of c_{1-} is determined by the following normalization condition $\int_0^\infty \left(u^2(r) + w^2(r)\right) r dr = 1$.

3. Numerical and graphic illustrations

Now we present some numerical and graphic illustrations in addition to the analytical results for the ground and first excited states in the particular cases $m = 1, m = -2$ at fixed $s = 0.05$.

Tables show the energies ϵ for different values of the Rashba parameter a, the well depth v and the magnetic field b .

Table 1: Energy levels for $m = 1$.

	$v = 50$				$v = 100$			
b	$a = 1$		$a = 2$		$a = 1$		$a = 2$	
0	10.23	20.31	7.97	20.73	11.16	22.08	8.85	22.59
0.5	11.33	22.50	8.84	23.09	12.25	24.24	9.73	24.94
1	12.65	24.95	9.92	25.70	13.55	26.64	10.81	27.53
1.5	14.18	27.68	11.23	28.52	15.05	29.29	12.08	30.32
2	15.93	30.67	12.74	31.54	16.74	32.18	13.56	33.32
2.5	17.88		14.47	34.68	18.62	35.30	15.23	36.47
3			16.39	37.92	20.68	38.65	17.08	39.75
3.5			18.49		22.90	42.20	19.10	43.11
4			20.76		25.27	45.94	21.28	46.47
4.5			23.16		27.77		23.61	49.82
5			25.70				26.07	53.17
5.5							28.65	56.57
6							31.32	60.10

Table 2: Energy levels for $m = -2$.

	$v = 50$				$v = 100$			
b	$a = 1$		$a = 2$		$a = 1$		$a = 2$	
0	10.23	20.31	7.97	20.73	11.16	22.08	8.85	22.59
0.5	9.36	18.41	7.33	18.63	10.26	20.18	8.18	20.47
1	8.71	16.79	6.89	16.79	9.57	18.52	7.70	18.60
1.5	8.26	15.45	6.66	15.21	9.08	17.12	7.40	16.98
2	8.02	14.37	6.61	13.91	8.77	15.96	7.29	15.59
2.5	7.96	13.56	6.74	12.87	8.63	15.05	7.33	14.45
3	8.08	12.99	7.01	12.08	8.66	14.36	7.53	13.55
3.5	8.34		7.42	11.53	8.84	13.90	7.86	12.87
4			7.94	11.21	9.15	13.64	8.31	12.41
4.5			8.55	11.09	9.58	13.58	8.86	12.15
5			9.24	11.18	10.11	13.70	9.50	12.08
5.5			9.98	11.43			10.20	12.19
6			10.77	11.84			10.95	12.46

Figures demonstrate the examples of continuous radial wave functions for $v = 100, a = 2$, $b = 5$. Solid lines correspond to the functions $u(r)$ and dashed lines correspond to the functions $w(r)$. We see that the radial wave functions rapidly decrease outside the well. The values of coefficients are $c_{1-} = -1.12025, c_{1+} = 14.2515, c_{2-} = -50929.1$ and $c_{2+} = 15539.3$ in the case of Fig. 1 and $c_{1-} = 0.21402, c_{1+} = 8.36721, c_{2-} = 102096$ and $c_{2+} = -7322.33$ in the case of Fig. 2.

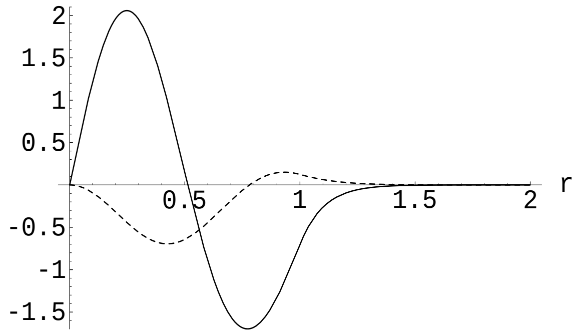

FIG. 1: Radial wave functions for $m = 1, e = 53.1715$.

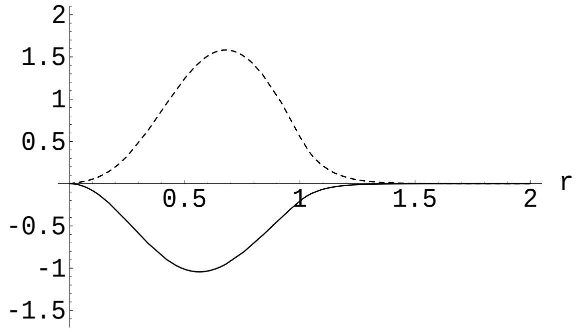

FIG. 2: Radial wave functions for $m = -2, e = 12.0827$.

4. Conclusion

So, we have constructed new exactly solvable and physically adequate model to describe the behavior of electron in a semiconductor quantum dot with account of the Rashba spin-orbit interaction and the external magnetic field

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