Rashba coupling in quantum dots in the presence of magnetic field

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We present an analytical solution to the Schrödinger 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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I. INTRODUCTION

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

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

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

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

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.

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 \( \rho < \rho_0 \), \( V_c(\rho) = V = \text{constant} \) 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).

II. ANALYTICAL SOLUTIONS OF THE SCHRODINGER 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

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

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Here $M_e$ is the electron mass. As it was shown in [5, 6], equation (1) permits the separation of variables

\[ \Psi_m(r, \varphi) = u(r)e^{im\varphi} \begin{pmatrix} 1 \\ 0 \end{pmatrix} + w(r)e^{i(m+1)\varphi} \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad m = 0, \pm 1, \pm 2, \ldots \]  

(5)
due to conservation of the total angular momentum $L_z + \frac{\hbar}{2} \sigma_z$. We have the following radial equations

\[
\begin{align*}
\frac{d^2u}{dr^2} + \frac{1}{r} \frac{du}{dr} + (\epsilon - v)u - \frac{m^2}{r^2}u - 2bmu - b^2r^2u - 4sbw &= a \left( \frac{dw}{dr} + \frac{m+1}{r}w + bw \right), \\
\frac{d^2w}{dr^2} + \frac{1}{r} \frac{dw}{dr} + (\epsilon - v)w - \frac{(m+1)^2}{r^2}w - 2b(m+1)w - b^2r^2w + 4sbw &= a \left( -\frac{du}{dr} + \frac{m}{r}u + bru \right). 
\end{align*}
\]

(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 [5] we use the substitutions

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

(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

\[ M(\alpha, \beta, \xi) - \frac{dM(\alpha, \beta, \xi)}{d\xi} = \frac{\beta - \alpha}{\beta} M(\alpha, \beta + 1, \xi), \]

\[ (\beta - 1 - \xi)M(\alpha, \beta, \xi) + \xi \frac{dM(\alpha, \beta, \xi)}{d\xi} = (\beta - 1)M(\alpha - 1, \beta - 1, \xi) \]

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

\[ u_1(r) = \exp \left( \frac{-br^2}{2} \right) (\sqrt{br})^{|m|} (c_1 - f_1 - (r) + c_1 + f_1 + (r)), \]

\[ w_1(r) = \exp \left( \frac{-br^2}{2} \right) (\sqrt{br})^{|m+1|} \left( \frac{a}{2\sqrt{b}} \right) (c_1 - g_1 - (r) + c_1 + g_1 + (r)), \]

(9)

where

\[ f_{1 \mp}(r) = M(m + 1 - k_{1 \mp}^2, m + 1, br^2), \]

\[ g_{1 \mp}(r) = \left( \frac{k_{1 \mp}^2}{m + 1} \right) M(m + 1 - k_{1 \mp}^2, m + 2, br^2) \]

(10)

for $m = 0, 1, 2, \ldots,$

\[ f_{1 \mp}(r) = M(1 - k_{1 \mp}^2, -m + 1, br^2), \]

\[ g_{1 \mp}(r) = m \left( -k_{1 \mp}^2, -m, br^2 \right) \]

(11)

for $m = -1, -2, -3, \ldots$ and

\[ k_{1 \pm} = \frac{1}{4b} \left( \epsilon + \frac{a^2}{2} \pm a \sqrt{\epsilon + \frac{a^2}{4} + \left( \frac{4b}{a} \right)^2 (s - 1/2)} \right). \]

(12)
Here $c_{2-}$ and $c_{2+}$ 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

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

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

of the confluent hypergeometric functions $U(\alpha, \beta, \xi)$ of the second kind [3] it is simply to get the suitable real solutions of the radial equations:

$$u_2(r) = \exp\left(\frac{-br^2}{2}\right)(\sqrt{br})^{|m|}(c_{2-}f_{2-}(r) + c_{2+}f_{2+}(r)),$$

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

where

$$f_{2\mp}(r) = \frac{\sqrt{\mp 1}}{2}(U(m + 1 - k_{2\mp}^-, m + 1, br^2) \mp U(m + 1 - k_{2\mp}^+, m + 1, br^2)),$$

$$g_{2\mp}(r) = \frac{\sqrt{\mp 1}}{2}\left(U(m + 1 - k_{2\mp}^-, m + 2, br^2) \mp U(m + 1 - k_{2\mp}^+, m + 2, br^2)\right)$$

for $m = 0, 1, 2, \ldots$,

$$f_{2\mp}(r) = \frac{\sqrt{\mp 1}}{2}(U(1 - k_{2\mp}^-, -m + 1, br^2) \mp U(1 - k_{2\mp}^+, -m + 1, br^2)),$$

$$g_{2\mp}(r) = \frac{\sqrt{\mp 1}}{2}\left(U(-k_{2\mp}^-, -m, br^2) \mp U(-k_{2\mp}^+, -m, br^2)\right)$$

for $m = -1, -2, -3, \ldots$ and

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

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

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

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

$$u_1(1) - u_2(1) = 0, \quad w_1(1) - w_2(1) = 0, \quad u'_1(1) - u'_2(1) = 0, \quad w'_1(1) - w'_2(1) = 0$$

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

$$T_3(m, \epsilon, v, a, b, s) \begin{pmatrix} c_{1-} \\ c_{1+} \\ c_{2-} \\ c_{2+} \end{pmatrix} = 0$$

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

$$T_3(m, \epsilon, v, a, b, s) = \begin{pmatrix} f_{1-}(1) & f_{1+}(1) & -f_{2-}(1) & -f_{2+}(1) \\ g_{1-}(1) & g_{1+}(1) & -g_{2-}(1) & -g_{2+}(1) \\ f'_{1-}(1) & f'_{1+}(1) & -f'_{2-}(1) & -f'_{2+}(1) \\ g'_{1-}(1) & g'_{1+}(1) & -g'_{2-}(1) & -g'_{2+}(1) \end{pmatrix}.$$
Hence, the exact equation for energy $\epsilon(m, v, a, b, s)$ is

$$\det T_1(m, \epsilon, v, a, b, s) = 0.$$  \hspace{1cm} (22)

This equation is solved numerically.

The desired coefficients are

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

where

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

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

### III. 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 $\epsilon$ for different values of the Rashba parameter $a$, the well depth $v$ and the magnetic field $b$.

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 $c_{1-} = -0.443198, c_{1+} = 5.63821, c_{2-} = -20148.7$ and $c_{2+} = 6147.72$ in the case of Fig. 1 and $c_{1-} = -0.065795, c_{1+} = -2.5723, c_{2-} = -31387$ and $c_{2+} = 2251.07$ in the case of Fig. 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 | 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 | 34.68 | 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 | 20.75 | | 25.27 | 45.94 | 21.28 | 46.47 |
| 4.5 | 23.16 | | 27.77 | 49.82 |
| 5 | 25.70 | | 26.07 | 53.17 |
| 5.5 | | | 28.65 | 56.57 |
| 6 | | | 31.32 | 60.06 |
TABLE II: Energy levels for \( m = -2 \).

|       | \( v = 50 \)   |       | \( v = 100 \)  |
|-------|----------------|-------|----------------|
|       | \( b \) \( a = 1 \) | \( a = 2 \) | \( b \) \( a = 1 \) | \( a = 2 \) |
| 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 |

FIG. 1: Radial wave functions for \( m = 1, e = 53.1715 \).

FIG. 2: Radial wave functions for \( m = -2, e = 12.0827 \).
IV. 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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