TWO ELECTRONIC STATES IN A QUANTUM RING: MATHIEU EQUATION APPROACH

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Abstract. The problem of two-electronic states is considered for the case of thin GaAs quantum ring in the framework of adiabatic approximation. It is assumed that electrons are localized on a circle, and the Coulomb interaction between the electrons depends only on angular coordinates. The real Coulomb interaction is replaced by function which makes it possible the separation of relative motion and the motion of the center of mass. The Mathieu equation is obtained for the relative motion of electrons. The harmonic, anharmonic and the libration regimes of oscillations are discussed.

1. Introduction

Quantum dots (QD) are very perspective objects in respect of the application in innovative semiconducting devises as an active media [1]. There is an opportunity of fabricating structures with desirable properties due to the wide range of methods of flexible manipulation of energetic spectrum of QD electron [1, 2]. The properties of the energetic spectrum of charge carriers in QD are defined by the range of characteristics of a sample such as the geometry and the component structure of the materials of QD. The close relationship between the above mentioned factors with the properties of QD have been investigated theoretically and experimentally in many works which are devoted to spherical, cylindrical, ellipsoidal, pyramidal and other QD-s (see for example [3]-[10]). Recently ring-shaped nanostructures have been fabricated [11], where the radial motion of carriers is confined both with the inner and outer borders. The importance of detailed theoretical study of physical properties of such systems is in the generalizing character of obtained results as one can realize quantum wells and wires as well as QDs by the limiting processes. The construction of the realistic Hamiltonian of a system, as far as it is possible, is necessary for the description of processes in quntum rings (QR), which allows us to calculate certain characteristics of QR. One and two electronic states in QR have been first investigated theoretically in pioneering work of Chakraborty and Pietilainen [12], where authors have modelled the confining potential of QR by the off-center two-dimensional oscillator. In the framework of this model, Halonen and others [13] have discussed the optical absorption in QR in a magnetic field by the same off-center oscillator approximation, in the presence of repulsive scattering centers. In [14] authors have studied QR as electron spin beam splitters. They have showed that quantum interference and spin-orbit interaction, in a one-dimensional mesoscopic semiconductor ring with one input and two output leads, can act as a spin beam splitter. The effects of the Coulomb interaction on the energy spectrum and the magnetization of two electrons in a strained
In$_x$Ga$_{1-x}$As/GaAs ring-like nanostructures are analyzed with realistic parameters inferred from the cross-sectional scanning-tunneling microscopy data in [15]. Thereby, the theoretical study of two-electron states in QR has both academic and implicational value. It stimulates the further observations of this concept. In this work we present the theoretical model of two-electron states in a thin GaAs QR with the rectangular infinitely high confining potential. The condition of the small thickness of QR allows us to use the adiabatic approximation as a result of which the interaction of electrons becomes a function on angular coordinates only.

2. Theory
Let us consider a GaAs QR with a small width $R_1 - R_2 \ll \{R_1, R_2\}$, which contains two electrons. The influence of QR borders on electron states in radial direction is so strong that we can describe the radial states of each electron by one particle approximation. This assumption allows us to consider the electrons located on the same distance from the QR center and the energy of Coulomb interaction between the electrons as a function of polar angles $\varphi_1$ and $\varphi_2$ (Fig. 1). In this case the two-particle Hamiltonian is the following:

$$\hat{H}(1, 2) = \sum_{i=1}^{2} \left\{ \frac{-\hbar^2}{2\mu} \left( \frac{1}{\rho_i} \frac{\partial}{\partial \rho_i} \left( \rho_i \frac{\partial}{\partial \rho_i} \right) + \frac{1}{\rho_i^2} \frac{\partial^2}{\partial \varphi_i^2} \right) + V_{\text{conf}}(i) \right\} + V_{\text{Coul}}(\varphi_1, \varphi_2),$$

where $\mu$ is the effective mass of electron (for GaAs $\mu = 0.067m_e$), $V_{\text{conf}}$ is the confining potential in radial direction and can be expressed as follows:

$$V_{\text{conf}} = \begin{cases} 0, & R_1 \leq \rho \leq R_2, \\ \infty, & [\rho < R_1, \rho > R_2]. \end{cases}$$

The expression of the Coulomb interaction will be given later. Since the radial wave functions of electrons are expressed by the Bessel function of the first and the second kinds, then in the adiabatic approximation the total wave function can be presented as the following product

$$\Psi(r_1, r_2, \varphi_1, \varphi_2) = f_0(r_1) f_0(r_2) \Phi(\varphi_1, \varphi_2),$$

Figure 1. Quantum ring with two electrons.
where

\[ f_0 (r_i) = C_1 I_0 (\kappa_0 r_i) + C_2 Y_0 (\kappa_0 r_i), \quad (3) \]

\[ I_0 (x), Y_0 (x) \] are the Bessel functions of the first and the second orders respectively [16], \( \kappa = \sqrt{2 \mu E_0 / \hbar^2} \). \( E_0 \) is the energy of one particle of the ground state, which is determined from the boundary conditions

\[ \left| \begin{array}{cc}
I_0 (\kappa_0 R_1) & Y_0 (\kappa_0 R_1) \\
I_0 (\kappa_0 R_2) & Y_0 (\kappa_0 R_2)
\end{array} \right| = 0. \quad (4) \]

Note, that function \( f_0 (r) \) satisfies the radial equation

\[ -\frac{\hbar^2}{2\mu} \left( \frac{1}{\rho} \frac{d}{d\rho} \left( \rho \frac{d}{d\rho} \right) \right) f_0 (\rho) + V_{conf} (\rho) = E_0 f_0 (\rho). \quad (5) \]

Substituting (2) into (1) and using (5), for the angular wave function we obtain the following equation:

\[ -\frac{\hbar^2}{2\mu R_{eff}} \left( \frac{\partial^2}{\partial \varphi_1^2} + \frac{\partial^2}{\partial \varphi_2^2} \right) \Phi (\varphi_1, \varphi_2) + V_{Coul} (\varphi_1, \varphi_2) \Phi (\varphi_1, \varphi_2) = (E - 2E_0) \Phi (\varphi_1, \varphi_2) = \varepsilon \Phi (\varphi_1, \varphi_2), \quad (6) \]

where it is assumed, that the distances of the particles from the QR center are fixed:

\[ R_{eff} = \frac{R_1 + R_2}{2}. \quad (7) \]

and the following notation is made: \( \varepsilon = E - 2E_0 \).

Let us turn to the definition of the expression of the potential \( V_{Coul} (\varphi_1, \varphi_2) \) of electrons interaction. We deal with two particles on a circle interacting with the repulsive potential. On the other hand it is clear that this potential should depend only on the mutual location of the particles, i.e. on \( \varphi_1 - \varphi_2 \), and it should be an even function, as the replacement of particles should not affect on the Hamiltonian. Meanwhile if \( \varphi_1 - \varphi_2 = \pi \) then \( V_{Coul}(\varphi_1, \varphi_2)|_{\pi} = e^2/(2\varepsilon_d R_{eff}) \), and if \( \varphi_1 - \varphi_2 = \pi/2 \) then \( V_{Coul}(\varphi_1, \varphi_2)|_{\pi/2} = e^2/(\sqrt{2}\varepsilon_d R_{eff}) \) (\( \varepsilon_d \) is dielectric constant and for GaAs \( \varepsilon_d \approx 13 \)).

With the increase of \( \varphi_1 - \varphi_2 \) from \( \pi/2 \) to \( \pi \) the function \( V_{Coul}(\varphi_1, \varphi_2) \) should decrease monotonically.

In simple approximation this function can be presented in the form:

\[ V_{Coul}^{appr} (\varphi_1, \varphi_2) = \frac{e^2}{R_{eff}\varepsilon_d} \left\{ \frac{1}{\sqrt{2}} + \frac{\sqrt{2} - 1}{2} \cos (\varphi_1 - \varphi_2) \right\}. \quad (8) \]

Note, that the exact Coulomb function is as follows:

\[ V_{Coul}^{ex} (\varphi_1, \varphi_2) = \frac{e^2}{\sqrt{2}\varepsilon_d R_{eff}\sqrt{1 - \cos(\varphi_1 - \varphi_2)}}. \]

The graphical representations of \( V_{Coul}^{appr} (\varphi_1, \varphi_2) \) and \( V_{Coul}^{ex} (\varphi_1, \varphi_2) \) functions in the region \( (\pi/2, \pi) \) are presented in (Fig. 2). As follows from the figure the qualitative features of both functions are the same, and the maximal shift of the values of the two potentials is 0.027 (Fig. 3). Thereby, for the radial wave function we obtain the following equation:

\[ -\frac{\hbar^2}{2\mu R_{eff}} \left( \frac{\partial^2}{\partial \varphi_1^2} + \frac{\partial^2}{\partial \varphi_2^2} \right) \Phi (\varphi_1, \varphi_2) + \frac{e^2}{\varepsilon_d R_{eff}} \left\{ \frac{1}{\sqrt{2}} + \frac{\sqrt{2} - 1}{2} \cos (\varphi_1 - \varphi_2) \right\} \Phi (\varphi_1, \varphi_2) = \varepsilon \Phi (\varphi_1, \varphi_2). \quad (9) \]
Figure 2. Approximated (1) and exact (2) functions of Coulomb interaction (in units of $\frac{e^2}{\varepsilon d R_{\text{eff}}}$).

Figure 3. Difference between approximated and exact functions of Coulomb interaction (in units of $\frac{e^2}{\varepsilon d R_{\text{eff}}}$).

Let us insert new variables $\alpha$ and $\beta$, related to $\varphi_1$ and $\varphi_2$ by the expressions:

$$\alpha = \varphi_1 - \varphi_2, \quad \beta = (\varphi_1 + \varphi_2)/2.$$  \hfill (10)

In this case the variables in (9) separate and the wave function, can be expressed in the form of the following product:

$$\Phi (\alpha, \beta) = u (\alpha) v (\beta).$$  \hfill (11)

Applying the separation procedure one can define the functions $u (\alpha)$ and $v (\beta)$ from the equations

$$-\frac{\hbar^2}{\mu R_{\text{eff}}^2} \frac{d^2 u (\alpha)}{d \alpha^2} + \frac{e^2}{\varepsilon d R_{\text{eff}}} \left( \frac{\sqrt{2} - 1}{2} \cos \alpha \right) u (\alpha) = E_\alpha u (\alpha),$$  \hfill (12)

$$-\frac{\hbar^2}{4\mu R_{\text{eff}}^2} \frac{d^2 v (\beta)}{d \beta^2} = E_\beta v (\beta).$$  \hfill (13)

Here the following relation is taken into account:

$$(E_\alpha + E_\beta) = \varepsilon - \frac{e^2}{\sqrt{2} R_{\text{eff}}}.\hfill (14)$$

Inserting in the equation (13) the electron total moment of inertia $J_{\text{eff}} = 2\mu R_{\text{eff}}^2$ for the eigenfunctions and the eigenvalues of equation (13) we can write:

$$v (\beta) = \exp \left( \frac{im\beta}{\sqrt{2\pi}} \right), \quad E_\beta = \frac{\hbar^2 m^2}{2J_{\text{eff}}} (m = 0, \pm 1, \pm 2, \ldots).$$  \hfill (15)

Let us now consider equation (12). Making the following notations:
\[ \alpha = 2\phi, \quad \lambda = \frac{4\mu R_{\text{eff}}^2}{\hbar^2} E_\alpha, \quad 2q = \left( \frac{\sqrt{2} - 1}{2} \right) \frac{4\mu e^2 R_{\text{eff}}}{\varepsilon_d \hbar^2}, \]
we can transform 12 to the Mathieu equation [17]:
\[ \frac{d^2 u(\phi)}{d\phi^2} + (\lambda - 2q \cos 2\phi) u(\phi) = 0. \tag{16} \]
As the one dimensional equation (16) contains symmetrical potential energy with respect to the point \( \phi = 0 \), their solutions have to be either even or odd periodic functions. One can write these solutions in the form of the Fourier expansion
\[ u_+(\phi) = \sum_{j=0}^{\infty} A_{2j} \cos (2j\phi), \quad u_-(\phi) = \sum_{j=1}^{\infty} B_{2j} \sin (2j\phi), \tag{17} \]
where \( A_{2j}, \ B_{2j} \) are the expansion coefficients. It is known from the Mathieu equation theory [17] that even and odd solutions and hence the energy levels alternate. If \( \{a_{2j}\}_{j=0}^{\infty} \) is the ensemble of the even, and \( \{b_{2j}\}_{j=1}^{\infty} \) is the ensemble of the odd solutions with respect to \( \phi \), hence the following inequalities take place:
\[ a_0 < b_2 < a_2 < b_4 < a_4 < ... \tag{18} \]
Finally for the even and odd energy levels we obtain the expressions:
\[ E_{2j}^+ = \frac{\hbar^2 a_{2j}}{4\mu R_{\text{eff}}^2}, \quad E_{2j}^- = \frac{\hbar^2 b_{2j}}{4\mu R_{\text{eff}}^2}. \tag{19} \]
Taking into account electron spin, we obtain the singlet states corresponding to the even levels, as the spin part of the wave function is odd. In \(z\)–presentation by the Pauli matrix
\[ \hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \]
the asymmetric spin wave function can be written as
\[ \chi_A = \frac{1}{\sqrt{2}} \left\{ \xi(1) \zeta(2) - \xi(2) \zeta(1) \right\}, \tag{20} \]
where
\[ \xi = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad \zeta = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \]
For the odd levels spin part of the wave function is symmetric and hence, the total wave function is triplet with the spin wave functions
\[ \chi_S = \left\{ \xi(1) \xi(2), \ \zeta(1) \zeta(2), \ \frac{1}{\sqrt{2}} \left\{ \xi(1) \zeta(2) + \xi(2) \zeta(1) \right\} \right\}. \tag{21} \]
Thereby in the considered system the singlet and triplet levels alternate and we finally obtain for the energy spectrum the following expressions:
\[ E_{2j,m}^+ = \left( 2E_0 + \frac{\hbar^2 a_{2j}}{4\mu R_{\text{eff}}^2} + \frac{\hbar^2 m^2}{2J_{\text{eff}}} + \frac{e^2}{\sqrt{2}\varepsilon_d R_{\text{eff}}} \right). \tag{22} \]
\[ E_{2j,m}^- = \left( 2E_0 + \frac{\hbar^2 b_{2j}}{4\mu R_{\text{eff}}^2} + \frac{\hbar^2 m^2}{2J_{\text{eff}}} + \frac{e^2}{\sqrt{2}\varepsilon_d R_{\text{eff}}} \right). \tag{23} \]
3. Discussions of results

Now let us consider the behaviour of the system depending on the effective radius of QR. According to (16) the effective “depth” of the one dimensional well increases with the increase of $R_{\text{eff}}$ as $q \sim R_{\text{eff}}$. It can be shown from the Mathieu equation theory, that for $\alpha = \pi$ Mathieu equation reduces to the harmonic oscillator equation, with the eigenvalue:

$$E_n = \frac{\hbar^2}{\mu R_{\text{eff}}^2} \left( n + \frac{1}{2} \right) - \frac{q\hbar^2}{2\mu R_{\text{eff}}^2}.$$  \hspace{1cm} (24)

It is due to the small oscillations of diametrical electrons, as a result of the decrease of repulsive force, which is in its turn, the result of the increase of QR effective radius. That is why
these oscillations will be harmonic. As follows from (24) the effective frequency of oscillations decreases with the increase of $R_{\text{eff}}$ due to the weakening of the oscillation force. Only the Coulomb part of the spectra of $E_{2j_\text{Coul}}$ as a function of effective radius $R_{\text{eff}}$ (the second and the forth terms in (22) and (23), are shown on (Fig. 4). Here the solid lines correspond to the even states, when the dashed lines correspond to the odd states. Note that the curves corresponding to the different parities do not cross and they decrease monotonically with the increase of $R_{\text{eff}}$, because the distance between electrons becomes larger, leading to the weaker Coulomb interaction. Meanwhile it follows from the behaviour of the solutions of the Mathieu equation, the levels $E_{2j_\text{Coul}}^+$ and $E_{2j_\text{Coul}}^-$ are very close to each other. The diagram of the discrete levels for $R_{\text{eff}} = 200\,\text{Å}, 400\,\text{Å}, 600\,\text{Å}$ is shown on (Fig. 5). The dependence of the parameter $\lambda$ on $q$ for the $R_{\text{eff}}$ changing in the range from $100\,\text{Å}$ to $800\,\text{Å}$ is shown on (Fig. 6). The levels which have the energy with value smaller than $2q$ correspond to the anharmonic oscillations that transform to harmonic ones with the increase of $R_{\text{eff}}$. Concerning to the levels that lie above the value $2q$, we can insist that libration oscillations correspond to them. In this case electrons move all over the QR with small oscillations and feel each other weakly. For the levels with high energy the energy of Coulomb interaction is negligible and we deal with almost free electrons.

4. Conclusion
A model of two electrons in GaAs thin QR is presented, which allows us to apply the adiabatic approximation and reduce the initial Schrödinger equation to the angular one. The Schrödinger equation with Coulomb potential is not analytically solvable and, therefore, a new approximated potential is introduced, which has the qualitative behavior similar to the exact function in the region between 90 and 180 degrees. This approximation enables us to separate the variables in (9) and to reduce the the equation to the Mathieu equation. The singlet and triplet states of energy for two electronic system is discussed. Finally, three classes of electron oscillations are discussed: harmonic, anharmonic and libration.
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