**D⁻ Energy spectrum in toroidal quantum ring**

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**Abstract.** The structure of energy spectrum of the negative donor centre in a toroidal-shaped quantum ring with two different morphologies of the cross-section is analyzed. By using the adiabatic procedure we have deduced a one-dimensional wave equation with periodic conditions which describes the low-lying energy levels related to the electrons rotation around the symmetry axis. Our results are in good agreement with those previously obtained as the size of the ring cross-section tends to zero.

**Introduction**

Motivated by the possibility of finding new physical effects and novel technological applications to opto-electronics, many researches have begun to analyze quantum dots with diverse morphologies. Nanostructures in a toroidal-shape have become a focus of attention because their topology allow us to get special laboratories for the study the mesoscopy physics related to quantum interference effects, such as the Aharonov–Bohm effect [1,2] and persistent currents [3]. In addition, these nanostructures can be used to carry out theoretical studies aimed at finding out the effects on the few-particle energy spectrum when dimensionality is reduced up to one in a very narrow nanoring. In this sense, the two-electron exactly solvable problem was recently reported in the papers [4-5] and some devices based on InGaAs toroidal quantum rings (QRs) have been designed and realized [6–7]. One-electron into a single toroidal QR [8] or double concentric toroidal QRs [9] under the presence of the homogeneous magnetic field is the simplest system that one can study in these semiconductor nanostructures. The one-particle energy spectrum has been calculated by using the diagonalization method [8-9], while energy structure of neutral shallow donors [9-10] and D⁺ molecular complex[11], which are also examples of one-particle systems, have been analyzed by using variational method [10] and a quasi-exact solution based on the adiabatic procedure [11-12]. As a neutral donor D⁰ traps a second electron released by other neutral donor a negative-donor D⁻ is formed [13]. The importance of this D⁻ center is related to the possibility of studying the electron-electron (e-e) correlation effects under the strong confinement conditions. Taking into account that the energy spectrum of few-particle systems becomes strong depending on the quantum confinement and the morphology of the quantum dots [14], this work is concerned with the determination of the D⁻ center energy structure as its two electrons are constrained to be moved into a toroidal QR while the positive ion is located in any point along of the QR symmetry axis. In spite of the fact that several features of the two-electron QRs can be explained in a simple mode by using a strictly one-dimensional QR [4-5], we are interesting to explore the cross-section morphology effect on the D⁻ energy spectrum since the connection between of the QR shape with the e-e interaction is still subject of great research.

**Physical system and theoretical framework**

We consider two electrons with an effective mass $m^*$ that are forced to move inside a nanoscopic toroidal QR whose cross-section of the area $\pi R^2$ may be circular with the radius $R$, or a square with the side $h = \pi^{1/2}R$, and whose centreline, defined as a circle passing through symmetry centres of the

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torus cross-sections, has sufficiently large radius $R_c (R_c >> R_s)$. The electrons are electrically bound to the positive ion (donor centre) located on the torus symmetry axis at the distance $\xi$ measured from its symmetry plane. Configurations and parameters of the considered models are shown in figure 1.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure1.png}
\caption{Configurations of negatively charged donors in a toroidal quantum rings with circular and square cross-sections}
\end{figure}

The dimensionless Hamiltonian of $D^-$ centre in the presence of a homogeneous magnetic field $B (B = B_0 \hat{z})$ applied along the $z$-axis in cylindrical coordinates is given by the following expression:

$$
\hat{H} = \sum_{j=1}^{2} \left( -\Delta_j - i\gamma \frac{\partial}{\partial \phi_j} + \frac{1}{4} \gamma^2 \rho_j^2 - \frac{2}{|r_j - \xi|} + V(\mathbf{r}_j) \right) + \frac{2}{|r_1 - r_2|}
$$

(1)

where $\mathbf{r}_1$ and $\mathbf{r}_2$ are the vector electrons positions, $V(\mathbf{r}_j)$ is the confinement potential, equal to zero and infinite inside and outside the torus, respectively. The units of the length, the energy and the magnetic strength used in equation (1) are the effective Bohr radius, $a_0^* = \hbar^2/\epsilon m^* c^2$, the effective Rydberg $R_y^* = e^2/2 \epsilon a_0^*$, and the first Landau level energy $\gamma = eBh/2m^* c R_y^*$, respectively. To describe the electrons positions let us introduce a three-dimensional orthogonal coordinate system $(\phi, \mathbf{e}_r)$, where $\phi$ is the angle that defines the direction of the position vector $\mathbf{r}$ over centreline while the two-dimensional unit vector $\mathbf{e}_r$ identifies the electron position inside the given cross section. Inside the nanoring the electron position is therefore described by $r_j = R_s (\phi) + \mathbf{p}_j (\mathbf{e}_r)$

(2)

In the case when the centreline radius $R_s$ is much larger than the cross section radius $R_c$ the eigenvalues of the Hamiltonian (1), can be found by using the adiabatic approximation that allows us to decouple the fast transverse electron motion from the slow rotation around $z$-axis [11]. The low-lying energy levels in this approximation are eigenvalues of the following effective Hamiltonian:

$$
\hat{H} = -\frac{1}{R_s^2} \left( \frac{\partial^2}{\partial \phi_1^2} + \frac{\partial^2}{\partial \phi_2^2} \right) - i\gamma \left( \frac{\partial}{\partial \phi_1} + \frac{\partial}{\partial \phi_2} \right) + U_{\omega}(\phi_1 - \phi_2) + \frac{1}{2} \gamma^2 R_s^2 + \frac{2}{\sqrt{R_s^2 + \xi^2}} + E_0
$$

(3)

$$
U_{\omega}(\phi_1 - \phi_2) = \left| f_s(\mathbf{p}_{1a}) f_s(\mathbf{p}_{2a}) \right| \left( \frac{2}{\sqrt{4R_s^2 \sin^2(\phi_1 - \phi_2) + (\mathbf{p}_1 - \mathbf{p}_2)^2}} \right) \left| f_s(\mathbf{p}_{1a}) f_s(\mathbf{p}_{2a}) \right|
$$

(4)

Here $f_s(\mathbf{p})$ and $E_0$ are the exact wave function and the corresponding energy in an infinite barrier two-dimensional quantum well related to the electron motion along the cross-section. By using the substitution $\theta = 0.5(\phi_1 + \phi_2)$ and $\phi = \phi_1 - \phi_2$ the two-particle Hamiltonian (4) can be separated into center-of-mass, $\hat{H}_c$ and relative $\hat{H}_r$ terms:
\[ \hat{H} = \hat{H}_c + \hat{H}_r; \quad \hat{H}_c = -\frac{1}{2 R_c^2} \frac{d^2}{d\phi^2} - i \gamma \frac{d}{d\phi} + \frac{1}{2} \gamma^2 R_c^2 \frac{2}{\sqrt{R_c^2 + \xi^2}} + E_c; \quad \hat{H}_r = -\frac{d^2}{d\phi^2} + U_{nr}(\phi) \] (5)

The eigenfunctions of the Hamiltonian (5) are \( \Psi_{M,m,r}(\phi, \theta) = \exp(i M \theta) \Phi_{m,r}(\phi) \) being \( M \) and \( m \) the center of mass and relative angular quantum numbers \((M, m = 0, \pm 1, \pm 2, \ldots)\) and \( s = \pm \) the eigenfunction parity. The even solutions \((s = +)\) correspond to singlet states and the odd solutions \((s = -)\) correspond to triplet states. In our numerical work, we solve the wave equation \( \hat{H}_r \Phi_{m,r}(\phi) = E_s(\phi) \Phi_{m,r}(\phi) \) by using the trigonometric sweep method [16].

Results and discussion

In order to check the quality of our calculation method we first calculated normalized energies \( \tilde{E}(M, m, s) = R_c^2 (E_c(M) + E_r(m, s)) \) for two-electron model \((\xi \to \infty)\) with centreline radii \( R_c \), \( a_0^* \) and \( 20 a_0^* \) as \( R \to 0 \) and compare them with those obtained in reference 4 for two-electron one-dimensional ring. Results in Table 1 show an excellent concordance between two sets of results.

| \( E(0,0,0) \) | \( E(\pm 1,0,1) \) | \( E(\pm 2,0,0) \) | \( E(0,2,1) \) | \( E(\pm 1,1) \) |
|----------------|----------------|----------------|----------------|----------------|
| Our results    | 5.18 22.40   | 5.68 22.90    | 7.18 27.54    | 7.91 24.40    |
| Ref. 4         | 5.18 22.40   | 5.68 22.90    | 7.18 27.54    | 7.91 24.40    |

The total energies of the \( D^- \) located at the centre of torous \((\xi = 0)\) with the cross-section size parameter \( R_t = 0.5 a_0^* \) as functions of the torous centreline radius \( R_a \) for some low-lying levels are shown in figures 2 (for square and circular sections in left- and right-side panels, respectively)

![Figure 2](image)

Figure 2. \( D^- \) energies of some low-lying levels as functions of the centreline radius for two different morphologies of the torous cross-sections: square (left panel) and circular (right panel).

One can observe that energies are sensitive to the morphology of the QR cross-section, although its size is very small. Comparison of energies of \( D^- \) ion shows that in a torus with square cross-section they are always below that those in torus with circular-cross section. It is due to the fact that the averaged separation between electrons is larger and the effective potential given by (4) is deeper in torus with square cross-section than circular one. As a result, the experimental observation of the \( D^- \) centre is more probable in torus with square cross-section than in circular one, since the the
$D^-$ ground state energy is lower and the system is more stable against the dissociation. Also one can see that the greater the ring centreline radius the greater is the $D^-$ energy and the smaller are gaps between different levels, independently of the cross section morphology. It is due to the fact that the contributions in the total energy of terms corresponding to the centre of mass and relative motion are inversely proportional to the centreline radius, $M/R_2^2$ and $m/R_1^2$, respectively, both tends to zero as the radius increases. On the other hand, one can see, as the centreline radius decreases, the energies for all levels monotonically decrease whereas the ground state energy tends the well known value of $1.055\,\text{Ry}^*$ [15] which corresponds to an energy value reported for the $D^-$ in bulk. It is due to the Coulomb energy term is strongly dominated by attraction between the electrons and the positive ion.

In figure 3, we display the evolution of the $D^-$ energy levels with the positive ion position along the z-axis for a QR with square cross-section. Remarkable evolutions of these curves are the result of the strong competition between electron-electron repulsion and the electron-ion attraction energy terms. As the positive ion is beyond $12\,a_0^*$ from the centre of the toroidal ring, the attractive potential energy term becomes depreciable while the electron-electron repulsion term increases because the electrons are constrained to move into the ring. This is the reason by which all energy levels in figure 3 have positive values as $\xi > 12\,a_0^*$. In the region $\xi < 12\,a_0^*$, one can observe a substantial increase of the total energy accompanied of a notable variation in the slope of the curves, while the energy values for all levels become positive only from $\xi > 12\,a_0^*$. From this value, the energy undergoes a significant reduction due to the dominance of electron-electron interaction.

![Figure 3. Energies of some low-lying levels of on-axis $D^-$ in a quantum ring with square cross-section as function of the distance between the positive ion position to the center of ring.](image)

The dependence of some energies levels $E(M,m,s)$ with $|M| \leq 3$ on the magnetic field strength for a toroidal QR with mean radius $R = 4\,a_0^*$ and square cross-section of side $1\,a_0^*$ is shown in figure 4 for three different values of positive ion position, 0.0 (left-panel), 5.0 (center panel) and 50\,a_0^* (right panel), respectively. From these panels, we can see once again that the greater the positive ion distance the greater is the energy values and the presence of the magnetic field yields the splitting of the energy levels whose angular momentum $M$ has different signs. The behaviour of these curves is the result of the strong competition between the paramagnetic and diamagnetic terms in the Hamiltonian (5). The contribution of diamagnetic term is quadratic with the magnetic field strength while the paramagnetic field is linear. For this reason, as the magnetic field strength is small, all the curves are quasi-linear with a constant slope, being positive for $M>0$ and negative for $M<0$, and they takes a parabolic shape for large values of the magnetic field strength which makes that the all curves with $M<0$ take a minima for values of $\gamma$ equal to $|M|/R^2$ a very narrow cross-section. This fact is responsible of the well known Aharonov-Bohm effect [1-2] which corresponds to the oscillatory
behaviour of the lowest level energy as measure as the magnetic strength growing with period given by $1/R^2$. In the present case, where the mean radius is equal to $4a_0$ * this period is equal $0.0625a_0$ *

Figure 4  $D^-$ energy levels as a function of the magnetic field strength in a toroidal quantum ring with mean radius $R = 4a_0$ * and square cross-section of side $R_t = 1a_0$ *

Conclusions

In short, the negative charged donor energy levels in very narrow toroidal QRs with two different shapes are investigated. We have shown that $D^-$ energy structure is dependent on the QR’s cross-section morphology. Finally, at the limit cases when the positive ion position tends to infinity or the size of the cross-section tends to zero, our results are an excellent concordance with the exact solutions.

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