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D_2^+ Molecular Complex in Ring-Like Nanostructures: Hydrostatic Pressure and Electromagnetic Field Effects

M.R. Fulla[a,b], J.H. Marín[b], W. Gutiérrez[c], C.A. Duque[d] and M.E. Mora-Ramos[d,e,f]

[a]Institución Universitaria Pascual Bravo, AA 6564 Medellín, Colombia

[b]Escuela de Física, Universidad Nacional de Colombia, AA 3840, Medellín, Colombia

[c]Escuela de Física, Universidad Industrial de Santander, AA 678, Bucaramanga, Colombia

[d]Grupo de Materia Condensada-UdeA, Instituto de Física, Facultad de Ciencias Exactas y Naturales Universidad de Antioquia UdeA, Calle 70 No. 52-21, Medellín, Colombia

[e]Facultad de Ciencias, Universidad Autónoma del Estado de Morelos, CP 62209, México

[f]Física Teórica y Aplicada, Escuela de Ingeniería de Antioquia, AA 7516, Medellín, Colombia

In this work we investigate the energy states in a D_2^+ complex formed by the coupling of a conduction band electron and two donor centers in a quantum ring with rectangular cross-section. The influences of externally applied probes like electric and magnetic fields and hydrostatic pressure together with the change in the relative position between the two Coulombic centers are particularly studied, highlighting the important contribution of the repulsive inter-center interaction. The destruction of the Aharonov–Bohm oscillations of the ground state associated with the localization of the electron states in the system is discussed.

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1. Introduction

In the last few years, nanostructures based on semiconductor materials in a ring-shape have been a subject of both experimental and theoretical researches [1–8]. In this context, the quick development of fabrication technology of quantum rings (QRs) has triggered a strong interest on these nanostructures due to the possibility to develop novel devices that combining the optical and electronic properties [6, 7] could boost the development of the optoelectronic industry and particularly the field of quantum computing [8]. In the present work, we consider an off-axis D_2^+ molecular complex confined in a QR under the presence of crossed electric and magnetic fields as well as the hydrostatic pressure. By using the adiabatic approximation, we address in detail the incidence of these fields on the D_2^+ energy structure as well as the effect of donor position and electric field on the localized electron states.

The structure of this work is organized as follows. In Sect. 2, we obtain the basic formulae from the D_2^+ Hamiltonian in the framework of the adiabatic approximation. Section 3 presents the results and discussion. Finally, the conclusions are summarized in Sect. 4.

2. Theoretical framework

We consider a single GaAs toroid-like QR generated by revolving around the z-axis a small rectangle of height L and width $W = R_\mathrm{O} - R_\mathrm{I}$, being R_I and R_O the inner and outer QR radius, respectively. Two shallow donor impurities are located on the plane x–y at distances ξ_1 and ξ_2 from the QR z-symmetry axis and they are bound each other through an electron which is forced to move into the QR. Figure 1 shows a schematic picture of the model system. The study takes into account the influence of the hydrostatic pressure by introducing the corresponding dependences of the electron effective mass and the dielectric constant on P (in kbar): $m^*(P)/m_0 = 0.0665 + 5.7076 \times 10^{-4} P$; $\varepsilon(P) = 12.25 - 0.027P$. Dimensions change according to the expression $L(P) = L(0)[1 - (S_{11} + 2S_{12})]^{1/2}$; whereas the radial size is $R_{\mathrm{I,O}}(P) = R_{\mathrm{I,O}}(0)[1 - 2(S_{11} + 2S_{12})]^{1/2}$, and $\xi_{1,2}(P) = \xi_{1,2}(0)[1 - 2(S_{11} + 2S_{12})]^{1/2}$.

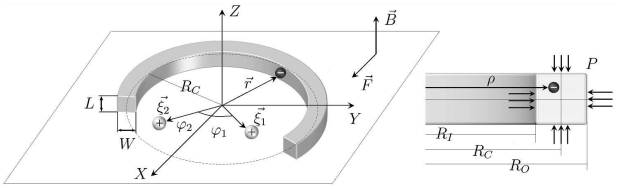

Fig. 1. Schematic 3D diagram of D_2^+ molecular complex with electron confined in toroid-like QR.

In the effective-mass approximation, the D_2^+ Hamiltonian under the effects of hydrostatic pressure, an x-direction-oriented electric field, $\boldsymbol{F}$, and in-growth-direction magnetic field, $\boldsymbol{B}$, can be written in cylindrical coordinates (ρ, φ, z) as follows:

$$
\begin{aligned}
H = &-\frac{\hbar^2}{2m^*(P)}\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right) + \frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2} + \frac{\partial^2}{\partial z^2}\right] \\
&+ \frac{\mathrm{i}e\hbar B}{2m^*(P)}\frac{\partial}{\partial\varphi} + \frac{e^2B^2\rho^2}{8m^*(P)} + V_\mathrm{c}(\rho, z, \varphi) \\
&+ |e|F\rho\cos\varphi - \sum_{j=1}^{2}\frac{e^2}{\varepsilon(P)\,|\boldsymbol{r} - \boldsymbol{\xi}_j|} + \frac{\eta e^2}{\varepsilon(P)\,|\boldsymbol{\xi}_2 - \boldsymbol{\xi}_1|}; \\
|\boldsymbol{r} - \boldsymbol{\xi}_j| &= \sqrt{\rho^2 + \xi_j^2 - 2\rho\xi_j\cos(\varphi - \varphi_j) + z^2}, \\
|\boldsymbol{\xi}_2 - \boldsymbol{\xi}_1| &= \sqrt{\xi_1^2 + \xi_2^2 - 2\xi_1\xi_2\cos(\varphi_2 - \varphi_1)}. \qquad (2.1)
\end{aligned}
$$

The confinement potential $V_c(\rho, z, \varphi)$ is assumed to be zero and infinite inside and outside the QR, respectively. An artificial parameter η has been included in order to analyze the D_2^+ energy structure by considering impurity–impurity interaction ($\eta = 1$) or leaving aside this interaction ($\eta = 0$). Thus, to calculate the D_2^+ molecular energy structure from the corresponding Schrödinger equation with Hamiltonian (2.1), we shall use an approximated method given that the attractive impurity-electron Coulomb interaction makes very hard to find an exact solution. Besides, a realistic self-assembled InGaAs QR is characterized by a very small height-to-center line radius aspect ratio, $(L/[0.5(R_I + R_O)] = L/R_C \ll 1)$. Bearing in mind this fact and considering for the sake of mathematical modeling very narrow QRs, whose widths are very small in comparison with their radii ($W/R_C \ll 1$), we can carry out a numerical procedure based on the adiabatic approximation (AA) [9]. In order to make more evident the possibility to use the AA approximation, the rescaling the variables ρ and z must be realized since their ranges of variation are strongly different from azimuthal variable. The substitutions announced above are, respectively, $\rho = R_I + W\tilde{\rho}$ and $z = L\tilde{z}$, where the new dimensionless variables $\tilde{\rho}$ and $\tilde{z}$ take values inside the QR between 0 to 1. Under these conditions the actual rectangular QR cross-section $W \times L$ has been mapped to other one with unitary area, where the new variables are now comparable allowing us to re-write the Hamiltonian (2.1) as

$$\tilde{H} = -\frac{\hbar^2}{2m^*(P)W^2}\frac{\partial^2}{\partial\tilde{\rho}^2} - \frac{\hbar^2}{2m^*(P)L^2}\frac{\partial^2}{\partial\tilde{z}^2} - \frac{\hbar^2}{2m^*(P)\left(R_I + W\tilde{\rho}\right)^2}\frac{\partial^2}{\partial\varphi^2} + \frac{\mathrm{i}e\hbar B}{2m^*(P)}\frac{\partial}{\partial\varphi} + \frac{e^2B^2\left(R_I + W\tilde{\rho}\right)^2}{8m^*(P)} + V_c(\rho, z, \varphi) + |e|F\left(R_I + W\tilde{\rho}\right) \times \cos\varphi - \sum_{j=1}^{2}\tilde{V}_j\left(\tilde{\rho}, \tilde{z}\right) + \frac{\eta e^2}{\varepsilon_2(P)\left|\boldsymbol{\xi}_2 - \boldsymbol{\xi}_1\right|}; \qquad (2.2)$$

with

$$\tilde{V}_j(\tilde{\rho}, \varphi, \tilde{z}) = e^2 \Big/ \Big[\varepsilon_1(P) \times \sqrt{(R_I + W\tilde{\rho})^2 + \xi_j^2 - 2(R_I + W\tilde{\rho})\xi_j\cos(\varphi - \varphi_j) + L^2\tilde{z}^2}\Big].$$

Equation (2.2) may be regarded as the corresponding Hamiltonian for three particles with hypothetical masses $2m^*(P)W^2$, $2m^*(P)L^2$, and $\approx 2m^*(P)R_C^2$, respectively, interacting by means of the potential $\sum_{j=1}^{2}\tilde{V}_j(\tilde{\rho}, \varphi, \tilde{z})$. The first two masses are much smaller than the other one, which allows us to decouple the fast transverse electron motion from the slow rotation motion around the z-axis by using the well-known adiabatic procedure. In consequence, the three-dimensional problem (2.2) is reduced to the following one-dimensional eigenvalue problem:

$$\tilde{H}\,\Phi(\varphi) = \left[-\frac{\hbar^2 A(\varphi)}{2m^*(P)}\frac{\partial^2}{\partial\varphi^2} + \frac{\mathrm{i}e\hbar B}{2m^*(P)}\frac{\partial}{\partial\varphi} + V_{\mathrm{rot}}^{(\eta)}(\varphi)\right] \times \Phi(\varphi) = E\,\Phi(\varphi),$$

$$V_{\mathrm{rot}}^{(\eta)}(\varphi) = \frac{e^2B^2C(\varphi)}{8m^*(P)} + |e|FD(\varphi)\cos\varphi - \sum_{j=1}^{2}U_j(\varphi) + \frac{\eta e^2}{\varepsilon_2\,(P)\left|\boldsymbol{\xi}_2 - \boldsymbol{\xi}_1\right|} + E_0(\tilde{\rho}, \tilde{z}), \qquad (2.3)$$

with

$$A(\varphi) = \int_0^1 \frac{\tilde{g}^2\,(\tilde{\rho}, \varphi)}{\left(R_I + W\tilde{\rho}\right)^2}\tilde{\rho}\,\mathrm{d}\tilde{\rho},$$

$$C(\varphi) = \int_0^1 \tilde{g}^2\,(\tilde{\rho}, \varphi)\left(R_I + W\tilde{\rho}\right)^2\tilde{\rho}\,\mathrm{d}\tilde{\rho},$$

$$D(\varphi) = \int_0^1 \tilde{g}^2\,(\tilde{\rho}, \varphi)\left(R_I + W\tilde{\rho}\right)\tilde{\rho}\,\mathrm{d}\tilde{\rho},$$

$$U_j(\varphi) = \int_0^1\int_0^1 \tilde{g}^2\,(\tilde{\rho}, \varphi)\,f^2\,(\tilde{z}, \varphi)\,V_j(\tilde{\rho}, \varphi, \tilde{z})\tilde{\rho}\,\mathrm{d}\tilde{\rho}\,\mathrm{d}\tilde{z}. \qquad (2.4)$$

To allow us to do the above procedure, we initially adopted a three-dimensional wave function as $\Psi(\tilde{\rho}, \varphi, \tilde{z}) = f_z(\tilde{\rho}, \varphi)g(\tilde{z}, \varphi)\Phi(\varphi)$, where $f_z(\tilde{\rho}, \varphi)g(\tilde{z}, \varphi)$ is the normalized ground state wave function electron in an infinite two-dimensional square quantum well whose lowest energy value is $E_0(\tilde{\rho}, \tilde{z}) = [\pi^2\hbar^2/2m^*(P)](1/L^2 + 1/W^2)$. The function $\Phi(\varphi)$ describes the slow electron rotating motion around the z-axis and satisfies the boundary condition $\Phi(-\pi) = \Phi(\pi)$. The one-dimensional Schrödinger Eq. (2.3) with azimuthal effective potential $V_{\mathrm{rot}}^{(\eta)}(\varphi)$ describing the molecular rotation effects may be solved by means of a series expansion in terms of the eigenfunctions of the orbital angular momentum operator as

$$\Phi(\varphi) = \sum_{m=-N}^{N} c_m\,\mathrm{e}^{\mathrm{i}m\varphi}. \qquad (2.5)$$

Replacement of this equation into Eq. (2.3) yields a secular equation of order N for non-trivial solution, which allows us to obtain the corresponding energy eigenvalues.

3. Results and discussion

In Fig. 2 we show the calculated effective potential $V_{\mathrm{rot}}^{(\eta)}(\varphi)$ presented in Eq. (2.3). Results are shown for an asymmetric radial positioning of the two Coulombic centers, as functions of the electron angular variable for a fixed difference of the angular coordinates of the two centers: $\Delta\varphi = \varphi_2 - \varphi_1 = \pi$ (a,b), and for fixed relation of the relative distances of the two centers from the origin, changing $\Delta\varphi$ (c,d). We are considering no electric or magnetic fields applied and two values of the hydrostatic pressure (0 and 30 kbar). Besides, we present the effective potential energy outcome in two distinct cases: $(\eta = 0)$ (a,c) and $(\eta = 1)$ (b,d).

It can be noticed that the effect of a nonzero applied pressure is to lower the energy as the result of the reduction in the overall size of the system, the increase of

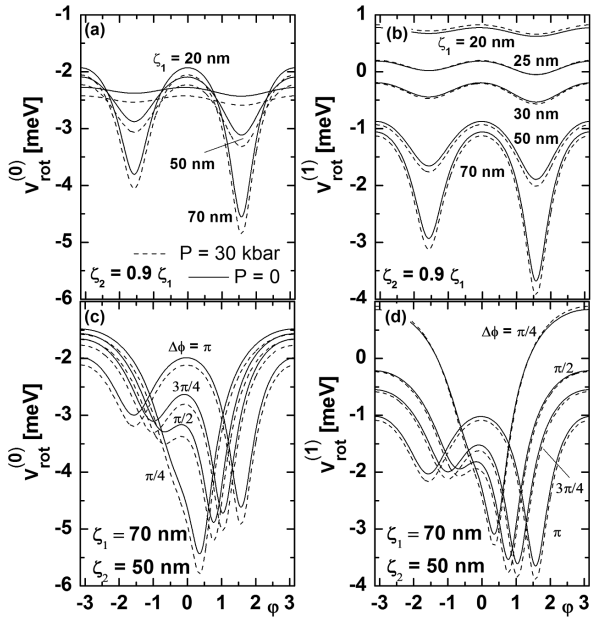

Fig. 2. Effective potential energy of the electron in a GaAs D_2^+ quantum ring complex as a function of the electron angular in-plane position (see detailed description in the text above). In all the figures, calculations are with $\Delta\varphi = \pi$, $L = 2$ nm, $F = 0$, $B = 0$, $R_c = 100$ nm, and $W = 10$ nm.

the electron effective mass, and the fall in the dielectric constant. All this reflects in the strengthening of the electrostatic coupling. We see that, as long as the donor atoms locate further from the inner QR wall (lower values of ξ_1 and ξ_2), the localization becomes less pronounced. Moreover, the connection of the inter-donor repulsion — which is merely an additional constant term in the renormalized Hamiltonian — leads, as expected, to a shifting upwards of the energy, weakening the Coulombic coupling of the electron and the D_2^+ complex. Such an effect becomes reinforced at nonzero pressure provided the rise in the strength of this repulsion associated with the size reduction and the decrease of the dielectric constant. One may even observe that, in the cases of near-origin center positions or small $\Delta\varphi$, the effect of pressure brings the energy curve above the zero pressure one for sufficiently large electron angular deviation. Up to our knowledge, this phenomenon has never been reported before in QR under hydrostatic pressure.

Figure 3 contains the variation of the electron state energy as a function of the applied magnetic field for the case $\eta = 0$. The same geometrical environment of the upper row graphs in Fig. 2 (parts (a) and (b)) is adopted, without applied electric field; but this time the radial distances of both centers from the origin are taken to be the same. The Aharonov–Bohm-like oscillations clearly appear. One observes the breaking in the appearance of anticrossings, for the lowest energies, as a consequence of the electron localization by the positive centers. For such localized states, the breaking of the degeneracy typical of the eigenstates of the orbital angular momentum is more apparent. It is possible to notice again the influence of the hydrostatic pressure in reinforcing the Coulombic coupling. In addition, we can observe that the vertical dotted line in the graphics coincides with the middle point of the curve for zero pressure whilst for the finite pressure it lies shifted rightward, thus showing the deformation of the oscillation induced by the pressure.

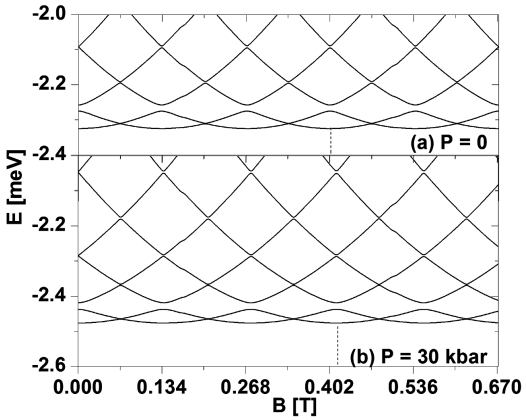

Fig. 3. Electron energies in a GaAs D_2^+ quantum ring complex as a function of the applied magnetic field for two values of the applied hydrostatic pressure (see a more detailed description in the text above). Calculations are with $\Delta\varphi = \pi$, $L = 2$ nm, $F = 0$, $R_c = 100$ nm, $R_I = R_O = 10$ nm, $\eta = 0$, and $W = 10$ nm.

On the other hand, Fig. 4 shows the same energy states depending on the magnetic field but, in this case, several values of the strength of an externally applied electric field are considered. The pressure value is set equal to 30 kbar and the remaining settings are the same discussed for the results presented in Fig. 3. This time, we readily notice a progressive destruction of the Aharonov–Bohm oscillations as long as the electric field intensity becomes higher. This is related with the expected correction to the energy posed by the field effect according to its orientation in the plane via the cosine of the angular electronic variable. In one limit case, the electric field pushes the electron towards the outer wall of the QR, whilst in the other the electron is attracted towards the inner wall. In this latter case, the effective electron–donor distance decreases and the Coulombic interaction becomes stronger. Thus, the degree of localization of the electron will be higher.

It is possible to confirm this by observing the effective potential $V_{rot}^{(0)}(\varphi)$ shown in Fig. 5. For small electric field strength values, there is a high probability of finding the electron at $\varphi = \pi/2$ and therefore the Coulombic centers share the electron with the same probability, that is, the electron is being collectivized by the two impurities. However, for an electric field strength greater than 0.01 kV/cm, the electrostatic force pushes the electron toward the neighborhood of the impurity located on $-x$-axis ($\varphi = \pi$) and, according to the second term at the

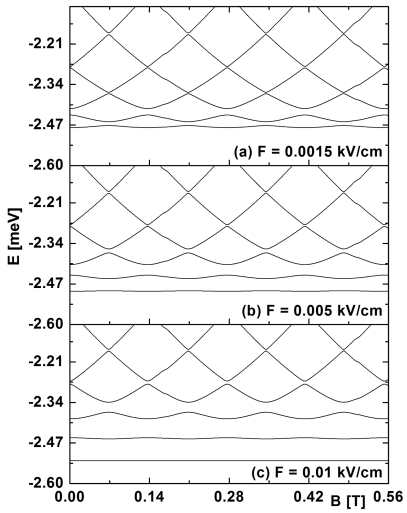

Fig. 4. Electron energies in a GaAs D_2^+ quantum ring complex as a function of the applied magnetic field for three values of the applied electric field (see description of Fig. 3 above). Calculations are with $\Delta\varphi = \pi$, $L = 2$ nm, $P = 30$ kbar, $R_c = 100$ nm, $R_I = R_O = 10$ nm, $\eta = 0$, and $W = 10$ nm.

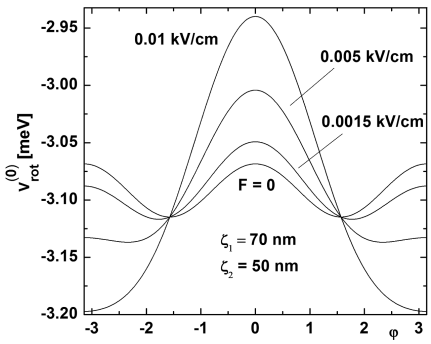

Fig. 5. The effective potential energy in a GaAs D_2^+ quantum ring complex as a function of the in-plane angular coordinate for different values of the applied electric field (see description of Fig. 3 above). Calculations are with $\Delta\varphi = \pi$, $L = 2$ nm, $B = 0$, $P = 30$ kbar, $R_c = 100$ nm, $R_I = R_O = 10$ nm, and $W = 10$ nm.

right of the lower equation in (2.3), the effective potential energy turns to be more negative since the Coulomb interaction is reinforced. As a consequence, localized states can appear more easily yielding a suppression of the AB oscillations because the impurities are practically isolated and the electronic collectivization between donors tends to be quenched.

4. Conclusions

In this work, we have studied some properties of the energy states in a D_2^+ complex involving conduction band electrons in a toroid-like GaAs quantum ring of rectangular cross-section. We have shown the effects that the changes in the geometrical configuration of the two donor centers, and/or the application of external probes like hydrostatic pressure and static electric and magnetic fields, have on the spectrum of such systems. One of the main results is the demonstration of the appearance of significant qualitative and quantitative modifications when the repulsive electrostatic interaction between the two ionized donor centers is taken into account in the calculation. In general, the application of hydrostatic pressure enhances the magnitude of the electron–donors coupling; but the inclusion of the inter-donor repulsion can even quench such a behavior for certain angular amplitudes of the electron motion. On the other hand, when there is an applied magnetic field, the hydrostatic pressure deforms the shape of the Aharonov–Bohm oscillations, and the presence of an external electric field can cause the destruction of these oscillations in the system.

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