Localized states induced by variations in the curvature of the path of an electron in a closed nanoscopic loop

J F Torres¹, N L Morales¹, J S Espitia¹, C J Páez¹, and W Gutiérrez¹
¹ Grupo de Investigación en Física Computacional de la Materia Condensada, Universidad Industrial de Santander, Bucaramanga, Colombia

E-mail: freddy-bmx83@hotmail.com

Abstract. We analyzed the effect of the curvature of the path on the energy spectrum of an electron confined in a closed nanoscopic loop in the presence of magnetic and electric external fields has been studied. The system was modeled using the stationary Schrödinger equation in the framework of the approximation of effective mass and enveloping function, which was solved using the finite element method. The closed loop has been modeled theoretically as a flat waveguide, whose width is small compared to the length of the path. These geometries allowed putting in evidence the variation in the confinement potential of the electron due to changes in the curvature. The variation of the electronic spectrum and the electronic densities for some low-lying energy states were analyzed as a function of the intensity of a magnetic field applied in the direction of growth and an electric field applied in the structural plane. The results demonstrate, with clarity, the high sensitivity of the electronic spectrum of a closed nanoscopic loop in the presence of changes in the curvature of the path, which translates into high sensitivity in electronic, magnetic and optical properties.

1. Introduction
There is no doubt that the growth of nanostructured materials is one of the greatest technological revolutions of recent times. In this context, the systems with the highest degree of confinement, such as quantum dots [1,3] and quantum rings [4–7], offer the greatest prospects for the appearance of new effects and for the development of new applications in optoelectronics. With the development of molecular-beam epitaxy and metal-organic chemical-vapor deposition [8,9], we can now control the size, composition and geometry of these semiconductor structures, with the precision of some nanometers. This refinement in crystal growth techniques has allowed the manufacture of nano-rings with a wide variety of morphologies, such as circular, oval and square [10,11]. About these latter there are very few theoretical research because the breaking of rotational symmetry imposes greater difficulty in solving the Schrödinger equation [12–14]. However, because they have C4 symmetry can become ideal candidates to study the correlation between structural symmetry and electronic properties in quantum systems; in addition, it allows to observe in a natural way the electronic localization due to the abrupt changes of curvature that occur in the corners of the closed loop. In this investigation, we analyze the Aharonov-Bohm oscillations of the electronic spectrum of a closed nanoscopic loop of a square shape using the finite element method. The system was modeled as a square ring with rounded corners,
considering different degrees of curvature, which allowed us to study the localizing effect that the potential of curvature has on the oscillations of the ground state energy by varying the magnetic field strength. The main motivation to study this closed loop with a square shape is to explore the electronic location in the four corners as a possible quantum gate, for potential applications in quantum information devices.

2. Materials and methods

2.1. System geometry

For the geometric description of the structure studied in this work, a generalized model was considered, which is shown in Figure 1. In this model a structure whose form is that of a closed loop of constant width and negligible height, located at $XY$ plane. This structure consists of some straight regions, as well as some curved regions limited by circumference segments of outer radius $r_{out}$ and inner radius $r_{inn}$. Also, the parameters were used $w$ and $r$ to define, respectively, the width of the loop and the radius of the center line of these curved regions (Equation (1) and Equation (2)). Finally, these equations are combined to express $r$ in terms of $w$ (Equation (3)); the latter to facilitate variations in the central radius since the width will remain constant for the structure studied.

$$w = r_{out} - r_{inn}$$  

$$r = \frac{r_{inn} + r_{out}}{2}$$  

$$r = r_{inn} + \frac{w}{2} = r_{out} - \frac{w}{2}$$

![Figure 1. General theoretical model of the geometry of a closed nanoscopic loop.](image)

2.2. System materials

To obtain results comparable with those of other authors, structures of $In_{0.55}Al_{0.45}As$ immersed in a matrix of $Al_{0.35}Ga_{0.65}As$ have been considered [4]. On the other hand, to facilitate the calculations, the existing mismatch in the joints of both the dielectric constant and the effective mass of the load carriers has been neglected and the values that correspond to the interior region of the nanostructure have been taken since the confinement causes the load carriers to be found mainly in this region. In addition, the ternary system of $In_{0.55}Al_{0.45}As$ has a dielectric constant $\varepsilon = 12.71$ and an effective mass for the electron $m^*_e = 0.076m_e$, where $m_e$ is the mass of the electron in vacuum. Also, the network constant of the nanostructure material is close to 0.6 nm.
2.3. Hamiltonian system
To facilitate the study of the Aharonov-Bohm effect (AB) in a uniform ring is convenient to use cylindrical coordinates \((\rho, \varphi, z)\), in addition to considering an infinite barrier potential, which is zero inside the ring and infinite outside of this one, as seen in Equation (4). On the other hand, the ring is in the presence of a homogenous external magnetic field \(B = B\hat{k}\), which is oriented along the axis of symmetry and defined through its vector potential \(A = \frac{1}{2}(B \times \rho)\), to its once, a homogeneous electric field \(F = F\hat{\iota}\) is applied in the \(X\) direction of the plane of the ring, defined by the electric potential \(\Phi = eF \cdot r\). Therefore, the Hamiltonian that adequately describes the behavior of an electron confined in a quantum ring (QR) and with structural confinement like infinite barrier potential is given by Equation (5).

\[
V_0 = \begin{cases} 
0 & \in QR \\
\infty & \notin QR 
\end{cases}
\]  
\[H = \frac{1}{2m_e^*}[p + eA]^2 + eF\rho \cos \varphi + V_0(\rho, \varphi)\]  
(5)

The definition of the linear moment vectors \(p = -i\hbar \nabla\) and magnetic potential \(A = \frac{1}{2}B\rho \hat{\varphi}\) allow us to obtain the Equation (6) and Equation (7).

\[
p \cdot A = -i\hbar A \cdot \nabla
\]  
(6)

\[
A \cdot p = -i\hbar A \cdot \nabla.
\]  
(7)

By substitution of \(p\) and the results obtained in the previous step in the Equation (5), the following result is obtained (Equation (8)).

\[
H = -\frac{\hbar^2}{2m_e^*}\nabla^2 - \frac{i\hbar e}{m_e^*}A \cdot \nabla + \left(\frac{e^2}{2m_e^*}\right)A^2 + eF\rho \cos \varphi + V_0(\rho, \varphi).
\]  
(8)

Finally, the vectors \(A = A\varphi \hat{\varphi}\) and \(\nabla = \nabla_\rho \hat{\rho} + \nabla_\varphi \hat{\varphi}\) defined in polar coordinates are replaced in Equation (8), finally arriving at the Hamiltonian expression that allows to study the effect of the curvature of the path in the spectrum energy of an electron Equation (9).

\[
H = -\frac{\hbar^2}{2m_e^*}\nabla^2 - \frac{i\hbar eB}{2m_e^*}\frac{\partial}{\partial \varphi} + \left(\frac{e^2B^2\rho^2}{8m_e^*}\right) + eF\rho \cos \varphi + V_0(\rho, \varphi)
\]  
(9)

2.4. Methodology
The Hamiltonian obtained in Equation (9) is a differential equation in partial derivatives (DEP) which does not allow a separation of variables, therefore, must resort to some numerical method to find their solution. In this work, we have made use of the Comsol computational tool based on a scheme of two-dimensional and triangular finite elements. Comsol offers the possibility of solving Equation (9) as a problem of eigenvalues in the form of coefficients, of the form, Equation (10).

\[
\lambda^2 c_a u - \lambda d_a u + \nabla \cdot (-c\nabla u - \alpha u + \gamma) + \beta \cdot \nabla u + au = f
\]  
(10)

In addition, Equation (9) has been divided between the electric charge unit \(e\) in order to express the energy in \(eV\). For all the above, the values of the coefficients of Equation (10) that were used to reproduce Equation (9) is Equation (11):
\[ \begin{align*}
    e_a &= 0 \\
    d_a &= 1 \\
    c &= \frac{\hbar^2}{2m_e^*} \\
    \alpha &= [0, 0] \\
    \gamma &= [0, 0] \\
    \beta &= \frac{ihB}{2m_e^*} [y, -x] \\
    a &= \frac{eB^2}{8m_e^*} (x^2 + y^2) \\
    f &= 0
\end{align*} \]

At this point, it became necessary to model the infinite barrier potential \( V_0(\rho, \varphi) \) of Equation \( (4) \) by imposing on Comsol the Dirichlet boundary condition, in which the wave function \( \psi \) cancels at the boundary. Finally, to perform the data processing, a script was designed in Matlab that reads the text document with the data exported from Comsol.

2.5. Loop architecture
To know the effect of the curvature of a closed loop of nanometric size on the energy properties of a confined electron, two different radius of average curvature have been considered, being one of them a multiple of the other, this in addition to allowing to demonstrate the existence of a structural confinement potential due to the curvature of the loop will also allow knowing the sensitivity of the system to changes in the curvature. Therefore, a series of transformations have been made on the general model of Figure 1 in such a way that, to take into account the previous considerations, the \( w = 10 \) nm width and the perimeter of these nanostructures will be fixed parameters, likewise radius of average curvature of 10 nm and 30 nm will be taken, these dimensions will allow obtaining nanoscale loops with sizes comparable to those obtained experimentally in [11]. The effect of the curvature of a closed nanometric loop in the form of a square with rounded edges will be studied. This can be understood as a circular QR that is divided into four equal parts, separated on each semiaxis a distance \( L \). Finally, these parts are joined through rectilinear regions of length \( L \) to give shape to three different cases: Table 1, Table 2 and Table 3. The last case to be studied is asymmetric since it does not keep symmetry with the \( X \) and \( Y \) axes.

**Table 1.** Geometrical parameters of a rounded square loop for a radius of average curvature \( r = 10 \) nm.

| \( x \) values | \( y \) values |
|-----------------|-----------------|
| \( x_1 = x_2 = x_3 = x_4 = \frac{r}{2} (6 + \pi) \) | \( r = 10 \) nm |

| \( y \) values | \( r \) values |
|-----------------|-----------------|
| \( y_1 = y_2 = y_3 = y_4 = \frac{r}{2} (6 + \pi) \) | \( r_1 = r_2 = r_3 = r_4 = r \) |

**Table 2.** Geometrical parameters of a rounded square loop for a radius of average curvature \( r = 30 \) nm.

| \( x \) values | \( y \) values |
|-----------------|-----------------|
| \( x_1 = x_2 = x_3 = x_4 = r \) | \( r = 30 \) nm |

| \( y \) values | \( r \) values |
|-----------------|-----------------|
| \( y_1 = y_2 = y_3 = y_4 = r \) | \( r_1 = r_2 = r_3 = r_4 = r \) |
Table 3. Geometrical parameters of an asymmetric rounded square loop for two radius of average curvature $R_1 = r = 10$ nm and $R_2 = 3r = 30$ nm.

| $x_1 = x_3 = y_1 = y_3 = \frac{r}{4} (16 + \pi)$ | $x_2 = x_4 = y_2 = y_4 = \frac{r}{4} (8 + \pi)$ | $r_1 = r_3 = r$ | $r_2 = r_4 = 3r$ |
|-------------------------------------------------|-----------------------------------------------|-----------------|-----------------|

3. Results

3.1. Potential for structural confinement

In Figure 2, a representation of the potential felt by the electron when it travels the loop along the intermediate path has been made, for three different configurations. It is interesting to note how for straight regions, where the curvature is zero, the potential is also zero, while in the corners of the structure true potential wells are created due to the existing curvature. The depth of these wells grows inversely with the square of the radius of curvature [15] and their width is related to the arc length of the corners.

![Figure 2](image1.png)

Figure 2. Potential for the structural confinement of an electron in a rounded quadrangular loop, as a function of the path length for two different radius of average curvature. (a) $r = 10$ nm, (b) $r = 30$ nm and (c) Both radius.

3.2. Effect of the magnetic field

The Figure 3 shows us the relationship that exists between the length of the path with the number of oscillations in energy and with the amplitude of them, this is a consequence of their geometric construction, since the three systems have the same perimeter. On the other hand, the decoupling of some energy states in the form of quadruples is due to the presence of the four potential wells. However, the appearance of pairs in Figure 3(c) is a consequence of the energetic difference presented by the curvature potential wells, the effect of the wells of the regions with the lower radius of curvature being more dominant, manifesting itself as an interference effect, which results in a more considerable amount of braids in the energy oscillations.

In the electronic density graphs of Table 4, the appearance of currents due to the application of a magnetic field is observed. On the other hand, it is possible to see the dominance of the curvature potential wells. This aspect is more marked on the ground state and the first degenerate state, which happens because these lower energy states are trapped inside the potential wells.
Figure 3. Energy as a function of the magnetic field for two different radius of average curvature. (a) $r = 10$ nm, (b) $r = 30$ nm and (c) Both radius.

Table 4. Electronic density of the lowest states for different magnetic field values $B$ in a rounded asymmetric square loop.

| Energy states | Magnetic field |
|---------------|----------------|
|               | $B=0.0$ (T)    | $B=0.2$ (T)    | $B=0.4$ (T)    |
| 1             | ![Image](image1) | ![Image](image2) | ![Image](image3) |
| 2             | ![Image](image4) | ![Image](image5) | ![Image](image6) |
| 3             | ![Image](image7) | ![Image](image8) | ![Image](image9) |
| 4             | ![Image](image10) | ![Image](image11) | ![Image](image12) |
| 5             | ![Image](image13) | ![Image](image14) | ![Image](image15) |
4. Conclusions
Our results show the appearance of variations in the confining potential experienced by a particle (electron) confined in a closed nanoscopic loop due to changes in the curvature of said structure. Using our method of solution based on finite elements, the emergence of right potential wells whose depth is inversely proportional to the square of the radius of curvature of the trajectory is corroborated.

The results obtained also show that the formation of potential wells along the loop, due to changes in the curvature, induce the appearance of molecular type spectra similar to those shown by nanoscopic rings in the presence of donor impurities or variations in the height of the structure. Likewise, it was observed how these curvature changes, depending on the symmetry of the structure, can inhibit the appearance of Aharonov-Bohm oscillations in the lower energetic levels, and therefore also inhibit the presence of persistent currents.

This study highlights the high sensitivity of the electronic spectrum to small variations in the curvature of a closed loop of nanometric size, which is indicative of how sensitive the optical and magnetic properties of these structures can be.

Acknowledgements
The authors are grateful to Prof. Dr. W Gutiérrez for his support and guidance in the preparation of this work.

References
[1] Ando T, Fowler A B and Stern F 1982 Rev. Mod. Phys. 54 437
[2] Bowler D R 2004 J. Phys. Condens Matter 16 R721
[3] Jacak L, Hawrylak P and Wójc A 1997 Quantum Dots (New York: Springer-Verlag)
[4] Aierken A, Hakkarainen T, Riikonen J and Sopanen M 2008 Nanotechnology 19 245304
[5] Jihoon H L, Zhiming M W, Morgan E W, Kushal C W, Garrido M, Stinaff E A and Salamo G J 2008 Cryst. Growth Des. 8 1945
[6] Heyn C, Stemmann A, Strelow C, Köppen T, Sonnenberg D, Graf A, Mendach S and Hansen W 2011 J. Nanoelectron Optoelectron 6 62
[7] Linares-García G, Meza-Montes L, Stinaff E, Alsalam S M, Ware M E, Mazur Y I, Wang Z M, Lee J and Salamo G J 2016 Nanoscale Res. Lett. 11 309
[8] Stern M B, Craighead H C, Liao P F and Mankiewich P M 1984 Appl. Phys. Lett. 45 410
[9] Waugh F R 1996 Phys. Rev. Lett. 75 705
[10] Boonpeng P, Jevasuwan W, Suraprapapich S, Ratanathammaphan S and Panyakesow S 2009 Microelectron. Eng. 86 853
[11] Schmidt O G 2007 Lateral Alignment of Epitaxial Quantum Dots (New York: Springer Berlin Heidelberg) p 92
[12] Sitek A, Tolea M, Nita M, Serra L, Gudmundsson V and Manolescu A 2017 Sci. Rep. 7 40197
[13] Gutiérrez W, García L F and Mikhailov I D 2013 Phys. B 421 63
[14] Marín J H, Gutiérrez W and Mikhailov I D 2019 Phys. E 111 98
[15] da Costa R C T 1981 Phys. Rev. A 23 1982