Eccentricity effects on the quantum confinement in double quantum rings

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Abstract

This work presents a theoretical study of the energy spectrum of GaAs/AlGaAs concentric double quantum rings, under an applied magnetic field directed perpendicular to the ring plane. The Schrödinger equation for this system is solved in a realistic model consisting of rings with finite barrier potentials. Numerical results show that increasing the magnetic field intensity leads to oscillations in the ground state energy which, in contrast to the usual Aharonov-Bohm oscillations, do not have a well defined period, due to the coupling between inner and outer rings states. However, when one considers an elliptical geometry for the rings, the energy spectra of the inner and outer ring states are decoupled and the periodicity of the oscillations is recovered.

Keywords: A. Semiconductors, C. Double Quantum Rings, D. Aharonov-Bohm Effect

1. Introduction

The increasing development of growth techniques has made it possible to fabricate nanometric structures which exhibit strong quantum confinement, such as quantum dots and quantum rings. Semiconductor quantum rings (QRs) have attracted much attention because they combine the optical properties of self-assembled nanostructures with unique features under applied magnetic fields originated by the ring topology, namely the Aharonov-Bohm (AB) effect. Recently, the growth of self-assembled GaAs/AlGaAs concentric double quantum rings has been reported, opening a new route to study AB oscillations and quantum interference effects. The electronic structure and excitonic properties of such systems were characterized by photoluminescence measurements in the absence of magnetic fields. Physical understanding and accurate modelling of such double rings are required for their future design and application, which stimulated the development of recent theoretical studies on circular concentric double quantum rings.

Previous theoretical works on semiconductor QRs have demonstrated interesting phenomena coming from non-circular geometries. The energy spectrum of a single QR with arbitrary shape was studied by Gridin et al., where they observed the existence of eigenstates localized at regions of maximum curvature. Later, Bruno-Alfonso and Latgé studied the more general case of non-uniform ring widths and arbitrary shapes of the centerline, where it was shown that even tiny variations of the ring width are able to produce quenching of the AB oscillations in the lowest energy levels. The specific case of elliptic single QRs was also considered by previous works, where it was shown that the low lying energy states are confined at the two regions of maximum curvature and their energies group in pairs exhibiting AB oscillations.

In this work, a time evolution method is used to calculate the energy eigenstates of electrons in GaAs/AlGaAs concentric double quantum rings, within the effective mass approximation. We will consider a model with finite barrier potentials, which is not limited to small perturbations and
which allows us to study rings with arbitrary sizes and shapes. For circular rings, our numerical results show that when the magnetic field is increased, energy oscillations are found, but they do not have a well defined periodicity, contrary to the AB oscillations found for single rings in the literature [23, 24]. Our results also show that the periodicity of the AB oscillations is recovered when an elliptic geometry is considered for one of the rings. In this case, the periodicity of the oscillations of the energy of the ground and first excited states is different from that found for the second and third excited states.

2. Theoretical Model

Our model consists of two concentric planar quantum rings, under an applied magnetic field $\vec{B} = B\hat{z}$, i.e., perpendicular to the ring plane. The Hamiltonian for such a system, using the symmetric gauge $\vec{A} = (-By/2, Bx/2, 0)$, is given by

$$H(\vec{r}) = T_x + T_y + V(x, y), \quad (1)$$

where

$$T_x = \frac{1}{2m} \left(-ih\frac{\partial}{\partial x} - \frac{eB}{2} \right)^2, \quad (2)$$

and

$$T_y = \frac{1}{2m} \left(-ih\frac{\partial}{\partial y} + \frac{eB}{2} \right)^2, \quad (3)$$

are the kinetic energy operators. The confinement potential is defined as $V(x, y) = 0$ within the ring region and $V(x, y) = V_e$ at the barrier region, where $V_e$ is the electron band offset. Figure 1 illustrates the two cases of double ring potentials discussed in this work: in Fig. 1(a), both inner and outer rings are circular, limited by radii $R_{1,i}$ and $R_{2,i}$ for the inner, and $R_{1,e}$ and $R_{2,e}$ for the outer rings. In Fig. 1(b), the circular outer ring is kept, but the inner ring is elliptic. The ellipses are defined by the eccentricity $\xi = a/b$, where $a$ and $b$ are the average distance between the limits of the inner ring in $x$ and $y$ directions, respectively, chosen to preserve the inner ring area.

Notice that in this simple model, the rings are assumed to be planar and spatially separated by a layer of a different material, represented by the potential barrier $V_e$ between them. In fact, the actual self-assembled double quantum rings reported in the literature have a finite height and are not completely spatially separated, namely, they are connected by their bottom. [11, 12] However, as the rings height is usually much smaller than their width, we assume that the confined electron is always in the ground state for the vertical confinement, so that the electronic transitions we will study in this work, related to the in-plane confinement, occur for energies lower than the first excited state energy of the vertical direction. As for the bottom connection, we point out that such a connection is a region of lower height separating the inner and outer rings. This narrowing in the vertical direction enhances the energy in the region between the rings and, consequently, the inner and outer rings are still effectively separated by a higher energy (barrier) region. Hence, we believe that our model, however simple it may be, still captures the most relevant physical aspects of the problem, at least in a qualitative way.

From the time dependent Schrödinger equation

$$ih\frac{\partial}{\partial t}\Psi(\vec{r}, t) = H\Psi(\vec{r}, t), \quad (4)$$

it is straightforward to find the time evolution of an arbitrary wavefunction $\Psi(\vec{r}, t)$ as

$$\Psi(\vec{r}, t + \delta t) = \exp \left[ \frac{ih}{\hbar} H\delta t \right] \Psi(\vec{r}, t). \quad (5)$$
The eigenstates of the Hamiltonian of Eq. (1) are then found by propagation of an arbitrary initial state in imaginary time domain $\tau = it$. The time evolution is performed by means of the split-operator technique. [21, 25] The differential operators in Eq. (2) and (3) are discretized, following a finite differences scheme. When $\tau \to \infty$, the initial state converges to the ground state of the system. Excited states are found by mixing this procedure with the Gram-Schmidt orthonormalization method. [26]

A qualitative analysis of the AB oscillations of the energy spectra of quantum rings can be made by considering a thin circular single quantum ring. In this case, neglecting any radial or perpendicular movement of the electron, i.e. considering that the electron moves only in the angular $\theta$-direction, with fixed position $\rho = R$ and $z = 0$ (cylindrical coordinates) the Hamiltonian can be written as

$$H^{\theta} = \frac{\hbar^2}{2mR^2} \left[ -i \frac{d}{d\theta} + \phi \right]^2.$$  \hfill (6)

where $\phi = \pi R^2 B$ is the magnetic flux threading the ring and $\phi_0 = e/\hbar$ is the quantum flux. The eigenfunctions of this Hamiltonian are easily found as $\psi_n(\theta) = \exp(in\theta)/\sqrt{2\pi}$, where $n = 0, \pm 1, \pm 2, \ldots$ is the angular momentum index, and the eigenenergies are

$$E_n^{(\theta)}(\phi) = \frac{\hbar^2}{2mR^2} \left[ n + \frac{\phi}{\phi_0} \right]^2.$$  \hfill (7)

The ground state energy as a function of $\phi$ given by Eq. (7) exhibits AB oscillations with period $\phi_0$ and its angular momentum index changes periodically at magnetic flux $\phi = (n + 1/2)\phi_0$. The results obtained by this simple approximation show that the period of the AB oscillations for an electron confined by a ring shaped potential of radius $R$ is $\Delta \phi = \phi_0/\pi R^2$, i.e. it is inversely proportional to the ring area. [27] This information will be useful for understanding the main features observed in the energy spectrum of double quantum rings in the following section.

3. Results and Discussion

We have calculated the energy spectrum for electrons in GaAs/Al$_{0.30}$Ga$_{0.70}$As double concentric quantum rings. For such a heterostructure, the electron band offset is $V_e = 262$ meV and the effective mass is assumed as $m_e = 0.067m_0$. [11]

Figure 2(a) shows the confinement energies of the four low-lying electron states in double circular rings as a function of the magnetic field. The inner ring is limited by internal and external radii $R_{1,i} = 230$ Å and $R_{2,i} = 330$ Å, respectively, whereas the outer ring has radii $R_{1,e} = 400$ Å and $R_{2,e} = 500$ Å. The dependence of the energy spectrum on the different rings widths was already studied in previous papers, [28, 29] therefore, in this work, we restrict ourselves to the analysis of the specific case of concentric rings with the same width. As the magnetic field strength increases, the energies exhibit non periodic oscillations, which differs from the energy spectrum of single rings reported in the literature, where periodic AB oscillations have been found [30, 12]. When both inner and outer rings exhibit circular symmetry, as in the present case, the energy spectrum of the double ring system can be obtained analytically. [12] Indeed, the numerically obtained energy spectrum in Fig. 2 is comparable to the analytical results presented in Fig. 4 of Ref. [12] or, equivalently Fig. 1 of Ref.
As we mentioned, in the system that we have considered, both the inner and outer rings have the same width, so that the eigenfunctions have no preferential ring to be confined in. Indeed, in the absence of tunnel coupling, each ring spans an energy spectrum that is periodic in $B$ with different periods according to Eq. (7), which are represented by the open and full symbols in the inset of Fig. 2, which illustrates the energy spectrum for two concentric rings delimited by a high potential barrier, i.e. with negligible coupling. The inter-ring coupling admix the two series of levels and destroys the periodic AB oscillations. Correspondingly, the resulting eigenstates delocalize between the two rings near an inter-ring resonance. This effect is illustrated in Fig. 2(b), which shows the calculated average radius $\langle \Psi_0 | r | \Psi_0 \rangle$ of the ground state. The average radius starts at the barrier region for $B = 0$, showing that in the absence of the magnetic field, the ground state is indeed distributed between the two rings. As $B$ increases, the average radius jumps between the inner and outer rings, leading to the non-periodic energy oscillation at low fields. However, for $B \gtrsim 2.6$, $\langle \Psi_0 | r | \Psi_0 \rangle$ stabilizes at the inner ring and, consequently, the ground state energy starts to oscillate periodically with $B$.

The previous results were obtained for two QRs with circular basis. However, as mentioned above, the eigenstates of single QRs are very sensitive to disorder, which are expected in actual samples. It is thus worth inquiring about the role of potential anisotropy on coupled QRs. To this end, we consider in the following the effect of a small deviation from a circular shape for one of the interacting rings. The electron energy spectrum for a system consisting of an elliptic inner ring and a circular outer ring is shown in Fig. 3. The inner ring presents eccentricities $\xi = 0.90$ (top) and $\xi = 0.95$ (bottom) (its average diameter is the same as the one in Fig. 1(a); see Ref. [21]). In this case, as only one of the rings is elliptic, it is hard to write the Hamiltonian in circular coordinates and find an analytical solution. More generally, analytical solutions cannot be obtained for arbitrary perturbation to the double quantum ring potential. Our method,
however, allows dealing with defects of arbitrary shape and strength.

The results in Fig. 3 show that as the eccentricity of the inner ring decreases, the ground \((E_0)\) and first excited \((E_1)\) states become more energetically separated from the second \((E_2)\) and third excited \((E_3)\) states. It can be clearly seen that the AB oscillations were recovered by the existence of an elliptic ring. Besides, the periodicity of the second and third excited states oscillations is different from the one found for the ground and first excited states. As the AB oscillations period is inversely proportional to the ring area, the higher period found for \(E_0\) and \(E_1\) oscillations indicates that these states are confined at the inner ring, while states corresponding to the energies \(E_2\) and \(E_3\) are then confined at the outer ring. Indeed, the period of oscillation for \(E_0\) and \(E_1\) \((E_2\) and \(E_3\)) is practically insensitive to \(\xi\), as obtained for a single QR, and equal to \(\Delta B \approx 1.75\) T \((0.7\) T), corresponding to AB oscillations for an electron confined in a \(R = \sqrt{\phi_0/\pi\Delta B} \approx 274\) Å \((433\) Å) quantum ring, according to Eq. (12), which is inside the inner (outer) ring region. The eigenfunctions \(\Psi_0\) and \(\Psi_2\) for the \(\xi = 0.90\) case are shown in Figs. 4(a) and 4(b), respectively, where we confirm that the former is confined in the inner (circular) ring, whereas the latter is confined in the outer (elliptic) ring. Similarly, the eigenfunctions \(\Psi_1\) and \(\Psi_3\) are localized within the inner and outer rings, respectively (not shown).

Figure 5: (a) Energies \(E_j\) and (b) average radii \(\langle r \rangle = \langle \Psi_j | r | \Psi_j \rangle\) of the four low-lying electron states as a function of the eccentricity of the inner ring.

Notice that even for deviations in the circular ring geometry as small as those shown in Figs. 3 and 4, the energy states in the inner and outer rings are already decoupled. It is then interesting to analyze how the coupled states in the inner and outer rings are already decoupled. To this purpose, in Fig. 5 we show the energy spectrum (a) and the average radii (b) of the four low-lying electron states as a function of the eccentricity of the inner ring. We observe that the eccentricity tends to decouple the two QRs. Moreover, the results in Fig. 5(b) demonstrate that in the circular double ring case, the ground state is confined in the inner ring region, as mentioned above, but the higher energy states are confined in the outer ring. However, as \(\xi\) decreases, the average radius of the first excited state decreases and eventually reaches the inner ring region for \(\xi \leq 0.95\). For smaller values of \(\xi\), the average radius of the ground and first excited (second and third excited) states converge to a value inside the inner (outer) ring region, as discussed earlier.

Finally, it is interesting to note that the two circular rings are strongly tunnel coupled, as evidenced by the strongly deformed energy spectrum in Fig. 2, as regards the spectrum we would obtain by a simple addition of the spectra of two independent rings. On the other hand, Fig. 3 shows that the eccentricity tends to decouple the two QRs. This result is not straightforward, since the eccentricity brings into play two opposite effects. Indeed, it introduces a region of higher curvature, which leads to an angular localization of the inner-related states. Such localized states are expected to less strongly interact with the more delocalized states of the outer ring (see Fig. 4). However, the inter-ring barrier potential is thinner in the angular region where the ground inner state is localized. This would on the contrary enhance the inter-ring interaction. The results in Figs. 3-5 show that the first effect dominates in the structure we consider here: even though the eccentricity locally favors inter-QR
coupling by a decrease of the tunnel barrier, it also render the coupling non-resonant by introducing a red-shift of the localized inner states that increases with decreasing $\xi$, as shown in Fig. 5.

The results presented in this paper regard only to one kind of perturbation of the geometry of the inner ring, namely, to deviations in the inner ring eccentricity. In this case, we demonstrated that the ground and first excited states are trapped in the higher curvature regions of the inner ring, decoupling inner and outer ring states. Other kinds of geometry perturbation in the inner ring are possible, which would produce regions with higher curvature \[19, 23\] or larger width \[51\] in this ring. In both cases, these regions would be more energetically favorable for the electrons confinement and thus, we expect that they would also be able to decouple the inner and outer ring states, otherwise coupled in the case of perfectly circular rings with the same width. However, the confirmation of this effect needs further investigation, and is left for future works.

4. Conclusions

A theoretical investigation of the electron confinement in double concentric quantum rings under applied magnetic fields was performed, for circular and elliptic rings. When circular rings are considered, the energy spectrum exhibits non-periodic oscillations as the magnetic field increases. However, periodic AB oscillations are found when one considers an elliptic inner ring, even when one deals with small eccentricities. Moreover, when one analyzes the periodicity of these AB oscillations, it can be seen that the eigenstates in such a system are spatially separated: ground and first excited states are confined at the elliptic inner ring, whereas the second and third excited states are confined at the circular outer ring.

Acknowledgments

We thank F. M. Peeters for a critical reading of the manuscript. This work has received financial support from the Brazilian National Research Council (CNPq), under contract NanoBioEstruturas 555183/2005-0, CAPES and PRONEX/CNPq/FUNCAP.

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