Position-dependent mass effects on a bilayer graphene catenoid bridge

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Abstract. We study the electronic properties of a position-dependent effective mass electron on a bilayer graphene catenoid bridge. We propose a position-dependent mass (PDM) as a function of both Gaussian and mean curvature. The Hamiltonian exhibits parity and time-reversal symmetry from the bridge symmetry. The effective potential contains the da Costa, centrifugal, and PDM terms which are concentrated around the catenoid bridge. For zero angular momentum states, the PDM term provides a transition between a reflectionless to a double-well potential. As a result, the bound states undergo a transition from a single state around the bridge throat into two states each one located at rings around the bridge. Above some critical value of the PDM coupling constant, the degeneracy is restored due to double-well tunneling resonance.

1 Introduction

Two-dimensional structures, as graphene \cite{1–3}, nanotubes \cite{4} and the phosphorene \cite{5} open a new venue to study the electron properties at low dimensional physics. The geometry of the graphene layer plays a pivotal role in the electronic structure. The curvature at the tip of a conical layer produces a topological phase \cite{6}, whereas helical strips induce chiral properties \cite{7–9}. Fluctuations of the geometry produce the so-called pseudomagnetic fields \cite{10}, whose effects can be seen at ripples \cite{11} and corrugated layers \cite{12}. The electron Hamiltonian on the surface can be obtained from the 3\textsuperscript{D} Hamiltonian by considering a small surface width \(\epsilon\), writing the Hamiltonian in the tangent and the normal coordinates, and then, taking the limit \(\epsilon \rightarrow 0\) \cite{13}. Starting with the 3\textsuperscript{D} Schrödinger Hamiltonian and applying this thin-layer squeezing method, one obtains a geometric potential, known as the da Costa potential \cite{14–17}. The geometric da Costa potential depends on the squared of the Gaussian and the mean curvatures and yields to an attractive potential. This method can also be extended to include external fields \cite{18}, spin in a Pauli equation \cite{19} and the Dirac equation on surfaces \cite{20}.

The geometry of the graphene layer can be used to develop new electronic devices. In Refs. \cite{21,22}, a bridge connecting a bilayer graphene was devised using a nanotube. To obtain a smooth bridge, the Ref. \cite{23} proposed a catenoid surface to describe the bilayer and the bridge using only one surface. This can be achieved due to the catenoid curvature which is concentrated around the bridge and vanishes asymptotically \cite{25}. The catenoid is a minimal surface, which is known to provide a stable graphitic structure \cite{26}.

In Ref. \cite{27}, we explored the effects of the geometry and external electric and magnetic fields upon the graphene catenoid bridge. The da Costa potential provides a reflectionless attractive potential, whereas the symmetry with respect to the \(z\) axis yields to a centrifugal repulsive term \cite{27}. The geometric potential exhibits a parity and time-reversal symmetry which holds under the action of the magnetic field but it is broken by the external electric field \cite{27}. The magnetic field produces a double-well potential which leads to bound states located at symmetric rings around the catenoid throat. The electric field creates a difference between the asymptotic values of the effective potential on the upper to the lower layer. This effect suggests that the catenoid bilayer bridge could be used as a diode \cite{27}.

Besides the geometric potential, it is expected that the surface curvature may also produce position-dependent mass effects. Indeed, the curvature breaks the homogeneity of the lattice which compose the layer, thus modifying the electron-effective mass. The PDM can be produced by \(p-n\) junctions driven by curvature \cite{28}, as well as phonon interactions \cite{29}. Although the position-dependent mass Hamiltonians in flat surfaces are widely studied \cite{30–33}, only recently an extension of the da Costa method including position-dependent mass effects on curved surfaces was proposed \cite{34}. The inclusion of an effective mass of form \(m^* \propto d^{-\alpha}\), where \(d\) is the nanotube diameter, on a corrugated
nanotube lead to significant modifications of the transport properties [34]. In a cylinder, the Gaussian curvature vanishes whereas the mean curvature is a constant $H = d^{-1}$. Thus, the position-dependent mass considered in Ref. [34] is proportional to a power of the corrugated mean curvature.

In this work, we study the effects of the position-dependent mass upon the electron on a catenoid bridge. In Sect. 2, we propose an isotropic position-dependent effective mass as a function of the Gaussian and the mean curvatures. Then, we analyze qualitatively the features of the effective potential, such as its behavior with respect to the parity, time-reversal symmetry, and hermiticity. In Sect. 3, we obtain the bound states and the corresponding energy spectrum. Final remarks and perspectives are outlined in Sect. 4.

2 Position-dependent mass electron on a catenoid surface

In this section, we introduce the geometry and the dynamics of the electron on the double-layer catenoid bridge considering the effects of a curvature-dependent mass. As shown in Fig. 1, the double-layer graphene bridge is realized as a smooth minimal surface (least area) joining the two planes. Near the bridge throat, depicted in Fig. 1, the symmetry about the $z$ axis and the vector $\hat{r}$ that locates a point on the surface of the catenoid in relation to the origin are shown.

After squeezing the electron wave function on a surface, the spinless stationary Schrödinger equation has the form

$$\frac{-\hbar^2}{2m^*} \nabla^2 \Psi + V_{dc} \Psi = E \Psi,$$  \hspace{1cm} (1)

where $\nabla^2 \Psi = \frac{1}{\sqrt{g}} \partial_a (\sqrt{g} g^{ab} \partial_b \Psi)$ is the Laplacian operator on the surface, $g^{ab}$ is the induced metric of the surface and $V_{dc} = -\frac{\hbar^2}{2m^*} (H^2 - K)$ is a potential induced by the surface curvature, known as the da Costa potential [14]. The geometric potential depends both on the mean curvature $H$ and the Gaussian curvature $K$ [14].

Recently, the electronic properties of the electron on the bilayer catenoid bridge were investigated assuming a constant effective mass $m^*$ [27]. Since the effective mass is also modified by the break of the lattice homogeneity driven by the curvature, we consider the modified position-dependent mass Schrödinger equation in the form [34]

$$(\mathcal{K} - V_{dc}) \Psi = E \Psi,$$  \hspace{1cm} (2)

where the position-dependent mass kinetic operator $\mathcal{K}$ is defined as

$$\mathcal{K} \Psi = -\frac{\hbar^2}{2m^*} \nabla^2 \Psi + \frac{1}{3} \nabla^2 \left( 1 \right) \Psi + \partial_i \left( \frac{1}{m^*} \right) \partial_i \Psi,$$  \hspace{1cm} (3)

and $m^* = m^*(x)$. Note that for a constant effective mass $m^*$ Eq. (1) is obtained.

Adopting a coordinate system formed from the meridian $u = u(z) = R \sinh (z/R)$ and the parallel $\phi$, where $u \in (-\infty, \infty)$ and the parallel $\phi \in [0, 2\pi)$, a point on the catenoid surface can be written as

$$\vec{r} = \sqrt{R^2 + u^2} \left( \cos \phi \hat{i} + \sin \phi \hat{j} \right) + R \sinh^{-1} (u/R) \hat{k},$$  \hspace{1cm} (4)

where $R$ the radius of the catenoid bridge throat.

In this coordinate system, the induced metric on the catenoid is $g_{uu} = 1$ and $g_{\phi\phi} = R^2 + u^2$, and the da Costa potential

$$V_{dc} = -\frac{\hbar^2}{2m^*} \frac{R^2}{(R^2 + u^2)^2}.$$  \hspace{1cm} (5)

It is worthwhile to mention that the da Costa potential $V_{dc}$ exhibits a parity-symmetrical potential well with respect to $u = 0$. In addition, the da Costa potential vanishes asymptotically, reflecting the asymptotic flat geometry of the catenoid. Note that the curvature leads to an attractive potential which tends to trap the electron around the origin.

The axial symmetry leads to the periodic behavior of the wave function in the form

$$\Psi(u, \phi) = \Phi(u) e^{i\nu \phi},$$  \hspace{1cm} (6)

where $\nu$ is the orbital quantum number. Substituting Eq. (6) into Eq. (2) yields to

$$-\frac{\hbar^2}{2m^*} \left[ \partial_u^2 \Phi + \frac{u}{R^2 + u^2} \partial_u \Phi - \frac{\nu^2}{R^2 + u^2} \Phi \right]$$
$$-\frac{\hbar^2}{6} \left[ \partial_u \left( \frac{1}{m^*} \right) + \frac{u}{R^2 + u^2} \partial_u \left( \frac{1}{m^*} \right) \right] \Phi$$
$$+ \frac{1}{R^2 + u^2} \partial_{\phi}^2 \left( \frac{1}{m^*} \right) \Phi$$
$$-\frac{\hbar^2}{2} \left[ \partial_u \left( \frac{1}{m^*} \right) (\partial_u \Phi) + \frac{i\nu}{R^2 + u^2} \partial_{\phi} \left( \frac{1}{m^*} \Phi \right) \right].$$
\[-\frac{\hbar^2}{2m^*} \frac{R^2}{(R^2 + u^2)^2} \Phi = E \Phi. \tag{7}\]

Equation (7) depends on the position dependence of the effective mass function $m^*$. In general, the effective mass may be anisotropic, as a result of a non-symmetric energy band \[34,35\]. In Ref. \[34\], the authors explored the electronic properties of position-dependent Schrödinger equation (2) on a nanotube. For that purpose, they considered $m^* \propto d^{-\alpha}$, where $d$ is the nanotube diameter \[34\].

Here, we propose that the curvature breaks the homogeneity of the system, and the consequence of such breaking leads to a modification in the effective mass of the particle moving along the surface of the system. Therefore, is natural to assume that the effective mass is related to the surface curvature. The surface curvature information is encoded in the second fundamental form $b_{ij}$ which satisfies \[25\]

\[
\frac{\partial^2 \tilde{r}}{\partial q^i \partial q^j} = b_{ij} \hat{n} + \Gamma^k_{ij} \frac{\partial \tilde{r}}{\partial q^k}, \tag{8}\]

where $\hat{n}$ is the unit normal vector to the surface and $\Gamma^k_{ij}$ are the Christoffel symbols. Since the catenoid geometry is isotropic, we adopt a position-dependent mass in the form

\[m^*(x) = m^* f(H, K), \tag{9}\]

being $m^*$ the effective mass of the electron in a flat graphene sheet and $f(H, K)$ is a particular function of the scalar invariants of the second fundamental form, the mean curvature $H = \text{Tr}(b_{ij})/2$ and Gaussian curvature $K = \text{det}(b_{ij})$. The presence of the both curvatures $H$ and $K$ not only leads to the position dependence of the effective mass $m^*$ but also guarantees that intrinsic and extrinsic deformations of the surface modifies the electron effective mass. It is worthwhile to mention that the position dependent mass considered in Ref. \[34\] satisfies Eq. (9) since the nanotube has $H = d^{-1}$ and $K = 0$, and so $m^*(x) = m^* H^\alpha$.

In this work, we consider an isotropic ansatz of form $m^*(x) = M(u)$ in the form

\[M(u) = m^* \left[1 + \lambda(H^2 - K)^\alpha \right], \tag{10}\]

being $\lambda$ a parameter given by the system, called coupling factor. The function $f(H, K) = 1 + \lambda(H^2 - K)^\alpha$ is dimensionless and it is built from the invariant term $(H^2 - K)$, known in the elasticity theory as the Wilmore energy \[36,37\]. For $\alpha = 1$, the coupling factor $\lambda$ has dimension of $\text{length}^2$ whereas the curvature term $(H^2 - K)$ has dimension of $\text{length}^{-2}$. Note that for the case of the catenoid (10) gives us

\[M(u) = m^* r(u), \tag{11}\]

where the function $r(u)$ is defined by

\[r(u) = 1 + \frac{\lambda R^2}{(u^2 + R^2)^2}. \tag{12}\]

Note that $M(u) \rightarrow m^*$ when $u \rightarrow \pm \infty$, in agreement with the fact that the catenoid is asymptotically flat when $u \rightarrow \infty$. When $u \rightarrow 0$ then $M(u) \rightarrow m^*(1 + \lambda/ R^2)$. Thus, $\sqrt{|\lambda|}$ measures a length of influence of the position-dependent mass effects.

The coupling constant $\lambda$ can assume positive or negative values. For $\lambda > 0$, the effective mass is augmented near the bridge throat and assumes the flat value $m^*$ asymptotically. For $\lambda < 0$, the curvature reduces the effective electron mass near the bridge. To prevent a vanishing effective mass, the coupling constant $\lambda$ should satisfy $\sqrt{-\lambda} \neq R$. For $\sqrt{-\lambda} < R$, the effective mass is everywhere positive. On the other hand, for $\sqrt{-\lambda} > R$ the effective mass is negative around the bridge throat interval $-R < u < R$ and positive for $|u| > R$. The effects of negative mass have been intensively studied in the last years in the context of Bose–Einstein condensation \[38\], acoustic systems \[39\], ion trapping \[40\], among others. However, we will not consider the possibility of negative mass here. The effects of the coupling constant $\lambda$ on the bound states will be explored in detail in the next section.

Using the curvature-dependent mass ansatz (11), the stationary Schrödinger equation along the meridian (7) reads

\[-\frac{\hbar^2}{2m^*} \left[ \frac{\partial^2 \Phi}{\partial u^2} + \frac{u}{R^2 + u^2} \partial_u \Phi - \frac{\nu^2}{R^2 + u^2} \Phi \right] - \frac{\hbar^2}{6} \left[ \frac{\partial^2 \left( \frac{1}{m^*} \right)}{\partial u^2} + \frac{u}{R^2 + u^2} \partial_u \left( \frac{1}{m^*} \right) \right] \Phi \]

\[-\frac{\hbar^2}{2} \partial_u \left( \frac{1}{m^*} \right) \partial_u \Phi - \frac{\hbar^2}{2m^*} \left( \frac{R^2}{(R^2 + u^2)^2} \right) \Phi = E \Phi \tag{13}\]

Note that Eq. 13 exhibits parity and time-reversal invariance, as a result of the catenoid geometric symmetries, as we can see from the acting of parity $P \tilde{u}(z)P = \tilde{u}(-z) = -\tilde{u}(z)$ and time-reversal $T \tilde{u}(z)T = \tilde{u}(z)$ operators upon $u(z)$. Nonetheless, the first-order derivative terms render the Hamiltonian non-Hermitian with respect to the meridian momentum $P_u := -i \partial_u$. The non-Hermiticity of the free electron Hamiltonian is not a problem, since the space-time reflection symmetry is preserved, the spectrum of the eigenvalues of the Hamiltonian is completely real \[41,42\]. Besides, there is an Hermitian equivalent Hamiltonian that can be achieved by a simple changing of variables. Considering the change in the wave function

\[\Phi(u) = \frac{1}{2} e^{\log(R^4 + \lambda R^2 + 2 R^2 u^2 + u^4) \frac{1}{2} (\log(R^2 + u^2))} y(u), \tag{14}\]
leads to an one-dimensional Hermitian Schrödinger-like equation
\[ -\frac{\hbar^2}{2M(u)} \frac{d^2y}{du^2} + V_{\text{eff}}(u)y = Ey, \]  
(15)
whose effective potential is given by
\[ V_{\text{eff}}(u) = V_c(u) + V_G(u) + V_\lambda(u), \]  
(16)
where \( V_c(u) \) is the centrifugal potential, \( V_G(u) \) is the geometric potential and \( V_\lambda(u) \) is the coupling potential, that are given by
\begin{align*}
V_c(u) &= \frac{\hbar^2}{2M(u)} \left[ \frac{\nu^2}{(R^2 + u^2)^2} \right], \\
V_G(u) &= -\frac{\hbar^2}{2M(u)} \left[ \frac{(2R^2 + u^2)^2}{4(R^2 + u^2)^2} \right], \\
V_\lambda(u) &= \frac{\hbar^2}{2M(u)} \times \left\{ \frac{2\lambda R^2 [4(R^2 - 2u^2) + (R^2 - 4u^2)(R^2 + u^2)^2]}{3[4(R^2 + u^2) + (R^2 + u^2)^3]^2} \right\}. 
\end{align*}
(17, 18, 19)

Although Eq. (15) resembles a Schrödinger equation, the operator on the left side \( \mathcal{H}y(u) = \tau(u)Ey(u) \) is not properly the Hamiltonian, since the “eigenvalue” depends on \( u \). By performing another wave function redefinition as \( y(u) = \frac{s_0}{\sqrt{\tau(u)}} \chi(u) \), being \( s_0 \) and arbitrary constant, we obtain the more familiar PDM Schrödinger equation [30–33]
\[ -\frac{\hbar^2}{2} \frac{d}{du} \left[ \frac{1}{M(u)} \frac{d\chi}{du} \right] + \tilde{V}_{\text{eff}}(u)\chi = E\chi, \]
(20)
and the effective potential is rewritten as
\[ \tilde{V}_{\text{eff}}(u) = V_c(u) + V_G(u) + \tilde{V}_\lambda(u), \]  
(21)
since, due to the redefinition of the wave function \( y(u) \), the coupling potential is rewritten as
\[ \tilde{V}_\lambda(u) = V_\lambda(u) + \frac{\hbar^2}{2M(u)} \left( -\frac{1}{2} \frac{r''(u)}{r(u)} + \frac{3}{4} \left( \frac{r'(u)}{r(u)} \right)^2 \right). \]  
(22)

Thus, the electron’s dynamics on a catenoid with Hamiltonian (13) is Hermitian equivalent to an electron under the action of the effective potential in (21). Moreover, the effect of curvature, PDM, and angular momentum are encoded in the effective potential. The equivalence between a \( PT \) symmetric non-Hermitian Hamiltonian and a Hermitian Hamiltonian has attracted much attention in last years [43–45]. Moreover, since (20) satisfies the continuity equation \( \frac{\partial |\chi|^2}{\partial r} + \frac{\partial j_r}{\partial u} = 0 \), the square of the wave function \( |\chi|^2 \) represents a true probability density.

Asymptotically, i.e., for \( u \rightarrow \pm \infty \), the effective potential in Eq. 21 vanishes and the PDM function reaches its asymptotic value \( M(U) \rightarrow m^* \), so that the respective asymptotic solution of Eq. (20) are of the form
\[ \chi(u) \approx A \cos(ku + \phi), \]
(23)
where \( k^2 = \frac{2m^*}{\hbar} \). Therefore, far from the bridge throat where the curvature effect vanish the electron behaves as free states. In the next section, we analyze the effect of the curvature and PDM on bound states near the bridge throat.

### 2.1 Qualitative analysis

Before obtaining the bound states and their respective spectra, let us discuss some qualitative features of the effective potential.

In Fig. 2, we show the effective potential given by Eq. 22, for \( R = 30 \text{Å} \), and \( \nu = 0 \), for some values of \( \lambda \). Equation 11 shows that the mass depends on coupling factor, \( \lambda \), and that in addition, \( \lambda \) can assume negative values, but not any negative value, there is a minimum limit value, which we call a critical coupling factor, \( \lambda_c \), from which the mass becomes negative, this critical value is given by \( \lambda_c = -R^2 \). For \( R = 30 \text{Å} \), the critical coupling factor \( \lambda_c = -900 \text{Å}^2 \), and it becomes deeper when \( \lambda \) assumes values close to the critical value, \( \lambda = \lambda_c \). In this case, the coupling effect suppresses the geometric effect. The effective potential decreases its depth when the \( \lambda \), having negative values, is increased until it reaches zero, as shown in the figure. A single-well is observed for \( \lambda = 0 \), this is the case when the effective mass is the same over the entire catenoid, \( M(u) = m^* = 0.03m_0 \). [27] When \( \lambda \) assumes positive values, the effective potential is drastically altered, generating two wells symmetrical in relation to the origin of the catenoid, in addition, the double-well becomes softer when \( \lambda \) takes on higher values, this behavior is shown in the results taken for \( \lambda = 10^3 \) and \( 10^5 \) \text{Å}^2. Under these conditions, the coupling is so intense that the geometric effect is suppressed. Therefore, the geometric effect is suppressed by the coupling effect in two limits, when \( \lambda \) tends to \( \lambda_c \) and when \( \lambda \) tends to infinity.

The effective potential for \( R = 30 \text{Å} \) and \( \nu = 1 \) is shown in Fig. 3. In this figure, in addition to the competition between the geometric and coupling potentials, discussed in Fig. 2, there is the centrifugal potential that significantly modifies the effective potential. When comparing the figures inserted in Figs. 2 and 3, we observe that the centrifugal effect is suppressed for \( R = 30 \text{Å} \), and it becomes deeper when \( \lambda \) assumes values close to the critical value, \( \lambda = \lambda_c \), in this case, the coupling effect suppresses the geometric effect. Therefore, the centrifugal effect is suppressed by the coupling effect in two limits, when \( \lambda \) tends to \( \lambda_c \) and when \( \lambda \) tends to infinity.
Fig. 2 The effective potential for $R = 30\,\text{Å}$ and $\nu = 0$ for some values of $\lambda$, obtained by Eq. 21

Fig. 3 The effective potential for $R = 30\,\text{Å}$ and $\nu = 1$ for some values of $\lambda$, obtained by Eq. 21

The effective potential takes the form of a barrier [27]. We also observed that when $\lambda$ assumes large positive values, the coupling effect changes the effective potential to form a double-well symmetrical in relation to the origin of the catenoid, suppressing the geometric and centrifugal effects. This behavior is shown in Fig. 3 for $\lambda = 10^5\,\text{Å}^2$, the same is observed in Fig. 2 for the same value of $\lambda$. Here, it is worth noting that both the geometric effect and the centrifugal effect are suppressed by the two-limit coupling effect, when lambda tends to $\lambda_c$ and when lambda tends to infinity, as discussed in Fig. 2.

The effective potential for $\nu = 0$ and $R = 70\,\text{Å}$ is shown in Fig. 4, for some values of $\lambda$. The increase in the radius of the catenoid throat increases the domain of the lambda values, considering that the minimum value of the critical lambda decreases to $-4900\,\text{Å}^2$. The behavior of the effective potential shown in Fig. 4 is similar to that of Fig. 2, that is, the potential has a deep well in the origin of the catenoid for $\lambda$ values close to the critical value. The depth of the well decreases when $\lambda$, having negative values, has its value increased to zero and finally when $\lambda$ increases, having its positive values, a double-well symmetrical in relation to the origin of the catenoid appears, and the increase in $\lambda$ decreases the depth of the double well. In both cases, the centrifugal potential is not present ($\nu = 0$), so the geometric potential competes with the coupling potential. Although qualitatively the results presented in Figs. 4 and 2 are similar, the radius of the catenoid throat is different. In this condition, increasing the radius value, $R$, decreases the geometric confinement on the effective potential, as studied in our recent work, see Ref. [27], as the critical lambda, $\lambda_c$, depends on the radius, the increase in the radius also causes the coupling potential to decrease its influence on the effective potential, but more smoothly, this is more evident when we compare the effective potentials with $\lambda$ values close to their respective critical lambdas, see the effective potential for $\lambda = -800\,\text{Å}^2$ in the figure inserted in Fig. 2, and for $\lambda = -4000\,\text{Å}^2$ in the figure inserted in Fig. 4.

The effective potential for $\nu = 1$ and $R = 70\,\text{Å}$ is shown in Fig. 5. This effective potential presents a qualitative behavior similar to the effective potential shown in Fig. 3. In both cases, the centrifugal potential is present ($\nu = 1$), and the results show that the increase in the radius, $R$, decreased both the geometric effect and the coupling effect on the effective potential, see the effective potential for $\lambda = -800\,\text{Å}^2$ in the figure inserted in Fig. 3, and for $\lambda = -4000\,\text{Å}^2$ in the figure inserted in Fig. 5.

3 Bound states

In the previous section, we discussed the effective potential generated by the surface of a catenoid of radius $R$, made of graphene, in which the effective mass of the electron depends on a coupling factor $\lambda$. In this sec-
tion, we will look at the electronic states accessible in these potentials.

For this, we solve numerically Eq. 20, using the finite difference method [46], for the effective potential given by Eq. 21, for some values of $R$ and $\lambda$. In the calculations, we use $m^* = 0.03m_0$, which is the effective mass of the electron on a single-layer graphene sheet and $m_0$ is the resting mass of the electron.

Figure 6 shows the bound states for $R = 30\,\text{Å}$ and $\nu = 0$ for four values of $\lambda$. We observe that the electronic state more confined is given by the effective potential for $\lambda = -850\,\text{Å}^2$ shown in Fig. 6a, the energy of this state is -26,020.21 meV and the probability density function shows that the electron has a high probability of being found close to the origin of the catenoid, see Fig. 6b. Making use of the angular symmetry of the catenoid and taking the width of the half-height of the probability density function, which is $\Delta u = 8.6\,\text{Å}$, we can visualize a probability cloud around the origin of the catenoid in the form of a ring, which we can call a probability ring. From what we see, this state is very localized, this is because the coupling factor chosen is very close to $\lambda_c$, in this situation the electron has a very small effective mass.

The probability ring is wider, $\Delta u = 100.8\,\text{Å}$, for $\lambda = 0\,\text{Å}^2$, so in this condition, the electron is less confined, as shown by the value of the energy level of the bound state which is -18.63 meV, as shown in Fig. 6c, d.

Two confined energy states appear for $\lambda = 10^3\,\text{Å}^2$, the first state is $-11.70$ meV and the second is $-0.24$ meV, see Fig. 6e. These states are not Gaussian functions, but states, called hybrids, that arise from the mixture of the states of the two wells symmetrical in relation to the origin of the catenoid [47]. The first state (dashed red line) presents a probability density function in the form of two Gaussians, practically overlapping, with their maximum separated from $\Delta u = 64.8\,\text{Å}$, one located at $u = -32.4\,\text{Å}$, and the other located at $u = 32.4\,\text{Å}$, see Fig. 6f.1. The cloud of probability associated with these states is in the form of two rings very close symmetrical in relation to the origin of the catenoid.

The second state (dotted blue line) presents also a probability density function in the form of two Gaussians, practically overlapping, but with their maximum separated from $\Delta u = 211.2\,\text{Å}$, one located at $u = -105.6\,\text{Å}$, and the other located at $u = 105.6\,\text{Å}$, see Fig. 6f.2. The cloud of probability associated with these states is also in the form of two rings very close symmetrical in relation to the origin of the catenoid, but wider which represents that this state is less confined in relation to the first.

Now, for $\lambda = 10^5\,\text{Å}^2$, these two hybrid states are practically degenerate, as they have almost the same energy value, $-6.19$ and $-6.17$ meV, see Fig. 6g, the probability density functions of the first hybrid state (red dotted line) and the second hybrid state (blue dotted line) are shown in Fig. 6h. The probability density function of each of these states takes the form of two Gaussians, one of the maximums being in $u = -90\,\text{Å}$, and the other is in $u = 90\,\text{Å}$. Again, taking into account the angular symmetry of the catenoid and the probability density function of the first state (red dashed line), Fig. 6h, we can visualize a probability cloud in the form of two rings located symmetrically in relation to the origin of the catenoid, with the width of each of these rings being $\Delta u = 124.9\,\text{Å}$. This probability density function expresses the fact that an electron initially located in one of the wells can pass from one side to the other of the catenoid, as it presents resonant tunneling. The same discussion holds for the second state as it has the same probability density function (blue dotted line) [47].

It is worth mentioning that for $\lambda = 10^6\,\text{Å}^2$ the states are degenerate with energy equal to $-2.26$ meV. This reflects what was said in the previous section, the effective potential becomes more shallow as the coupling factor increases, $\lambda$, consequently the energy of the connected states gets smaller and smaller to the point of ceasing to exist. In these conditions the effective mass of the electron is so large that the effective potential can no longer confine it, so an electron coming from infinity, on the surface of the catenoid, passes through the throat of the catenoid, experiences a phase shift in its wave function and goes on to infinity.

Figure 7 shows the bound states for $R = 30\,\text{Å}$ for four values of $\lambda$, however, we take in account the centrifugal potential, $\nu = 1$. We observe that the states become less localized when compared with the results, see Fig. 6, where the centrifugal potential is absent. When looking at Figs. 6a and 7a, we do not observe the influence of the centrifugal potential on the effective potential, because apparently, the potentials are very similar, and even the probability density functions have, approximately, the same width ($\Delta u = 9.2\,\text{Å}$), however, the energy value of the bound state is changed to $-24,206.83$ meV.

Figure 7c shows the energy of the bound state, for $\lambda = -600\,\text{Å}^2$, which is $-123.70$ meV, and the probability ring, located at the origin, has a width of $\Delta u = 28\,\text{Å}$.
Fig. 6 The bound states and their probability densities for a catenoid with radius $R = 30\text{Å}$ and $\nu = 0$. The solid black line represents the effective potential for: $a \ \lambda = -850\text{Å}^2$, $c \ \lambda = 600\text{Å}^2$, $e \ \lambda = 10^3\text{Å}^2$ and $g \ \lambda = 10^3\text{Å}^2$. The red dashed and blue dotted lines correspond to the first and second bound states and their probability densities, respectively.

Fig. 7 The bound states and their probability densities for a catenoid with radius $R = 30\text{Å}$ and $\nu = 1$. The solid black line represents the effective potential for: $a \ \lambda = -850\text{Å}^2$, $c \ \lambda = -600\text{Å}^2$, $e \ \lambda = 1.5 \times 10^4\text{Å}^2$ and $g \ \lambda = 10^5\text{Å}^2$. The dashed red and blue dotted lines correspond to the first and second bound states and their probability densities, respectively.

Å, as shown Fig. 7d. We observed that for values of $\lambda$ closer to $\lambda_c$, the electronic state is more confined.

No bound state is observed for $\lambda = 0\text{Å}^2$, because for $\nu = 1$, the effective potential is a barrier and not a well. This barrier is shaped like a Gaussian, whose height is 71.43 meV and its width is 35.71 meV [27].

Due to the presence of the orbital angular momentum, $\nu = 1$, the linked states were only obtained for values of $\lambda$ greater than $10^4\text{Å}^2$, then we calculate the effective potential for $\lambda = 1.5 \times 10^4\text{Å}^2$, for this configuration, two hybrid states are observed as shown in Fig. 7e, f, the energy of the first (dashed red line) and second (dotted blue line) states are $-0.72$ meV and $-0.33$ meV, respectively. The probability cloud, of the first state (dashed red line), is in the form of two rings, one located at $u = -63.6\text{Å}$ and the other located at $u = 63.6\text{Å}$, each ring having a width of $\Delta u = 134.8\text{Å}$. While the second (dotted blue line), the probability rings are located in $u = -66.0\text{Å}$ and $u = 66.0\text{Å}$, and the width of each one is $\Delta u = 147.6\text{Å}$.
Two hybrid states also appear for \( \lambda = 10^3 \), Fig. 7g, h, the energy of the first (dashed red line) and second (dotted blue line) states are \(-1.69\) meV and \(-1.66\) meV, respectively. Their probability rings are practically coincident and they are located at \( u = -92.4\) Å and \( u = 92.4\) Å, with the width of the rings being \( \Delta u = 150\) Å. These states are less confined compared to the states shown in Fig. 6g, h, where the centrifugal potential is absent, \( \nu = 0 \).

Figure 8 shows the bound states and their probability density functions for \( \nu = 0 \) and \( R = 70\) Å, for four values of the \( \lambda \). According to the results shown in Fig. 8, the increase in the radius of the catenoid decreases and even remove the bound state, as is the case for \( \lambda = 10^3\) Å². Therefore, increasing the radius of the catenoid decreases the effect of the geometric potential on the effective potential of the system. For example, for \( \lambda = -850\) Å², the energy of the bound state is \(-5.14\) meV, and the width of the probability density function is \( \Delta u = 168.4\) Å.

For \( \lambda = 0\) Å², the energy of the bound state is \(-3.42\) meV, and the width of the probability density function is \( \Delta u = 236.8\) Å. For \( \lambda = 10^3\) Å², one of the states seen in Fig. 6e is removed, and the remaining one has an energy of \(-2.63\) meV, with the width of the bound state being \( \Delta u = 312.0\) Å, see Fig. 8f.

The same hybrid states that appear for \( R = 30\) Å and \( \lambda = 10^5\) Å², for both \( \nu = 0 \) and \( \nu = 1 \), see Figs. 6 and 7, also appear for \( R = 70\) Å, as shown in Fig. 8g, h. However, they are less localized. The energy of the first state (dashed red line) is \(-1.97\) meV, and of the second (dotted blue line) is \(-1.87\) meV. Here, we notice a slight breakdown of degeneracy, although the probability density functions, which are shown in Fig. 8h, are overlapping. From the probability density functions, we can visualize two probability rings, one located at \( u = -140\) Å and the other at \( u = 140\) Å, being the width of each of these rings \( \Delta u = 219.2\) Å. These hybrid states become even less localized to take into account the orbital angular momentum, \( \nu = 1 \), for \( R = 70\) Å, as shown in Fig. 9g, h, in which the energy of the first state (dashed red line) is \(-0.19\) meV and the second state (dotted blue line) is \(-0.13\) meV. The probability cloud of the first state (dashed red line) is in the form of two rings, one located at \( u = -153.6\) Å and the other located at \( u = 153.6\) Å, each having a width of \( \Delta u = 299.2\) Å. For the second state (dotted blue line), the cloud of probability is also shaped like two rings, one located at \( u = -158.4\) Å and the other located at \( u = 158.4\) Å, each having a width of \( \Delta u = 313.6\) Å.

No state linked to \( \lambda = -850\) Å² is found when in addition to increasing the radius of the catenoid to \( 70\) Å, we take into account the centrifugal potential, \( \nu = 1 \).

The energy of the bound state for \( \nu = 1 \), \( R = 70\) Å, and \( \lambda = -4850\) Å², is \(-152.812.01\) meV, and the probability density function has a width equals to \( \Delta u = 9.2\) Å. Both the energy of the bound state and its probability density function are shown in Fig. 9a, b. As we can see, this state is strongly linked because the value of \( \lambda \) used is close to \( \lambda_c = -4900\) Å². The absence of the centrifugal potential (\( \nu = 0 \)) alters the energy of the bound state, to \(-154.638.10\) meV, even for a coupling potential so close to the critical \( \lambda_c \).

Increasing \( \lambda \) to \(-3000\) Å² the energy of the bound state is altered to \(-6.49\) meV, as well as, its probability density function, the width is \( \Delta u = 76\) Å, as shown the Fig. 9c, d.

Finally, for \( \lambda = 10^6\) Å², the energy of the first state (dashed red line) is \(-0.274\) meV and the second state (dotted blue line) is \(-0.273\) meV. The probability cloud of the first state (dashed red line) and the second state (dotted blue line) is overlapping. The two probability clouds are shaped like two rings, one located at \( u = -248.0\) Å and the other located at \( u = 248.0\) Å, each having a width of \( \Delta u = 395.2\) Å. The question of these states becoming less and less localized when the coupling factor increases, has been discussed previously in the text.

4 Final remarks and perspectives

We investigated the electronic states of a position-dependent mass (PDM) electron confined on the surface of a graphene catenoid bridge. In addition to the usual geometric potential, we considered a PDM mass as a function of the mean and the Gaussian curvatures.

The coupling between the curvature and the electron mass is controlled by a coupling constant \( \lambda \), which can take any value in the interval \( \lambda_c < \lambda < \infty \), where the critical value \( \lambda_c \) is given by \( \lambda_c = -R^2 \) and \( R \) is the radius of the catenoid throat.

The effective potential contains the usual geometric da Costa potential, the centrifugal term and the PDM corrections. Asymptotically, the effective potential vanishes and free states are allowed. Near the bridge throat, the effective potential is strongly dependent on the PDM parameter \( \lambda \). For \( \lambda_c < \lambda < 0 \), the potential exhibits an attractive volcano-like shape around the origin, regardless of the value of the angular momentum.

For \( 0 \leq \lambda < \infty \), the effective potential is rather dependent on the angular momentum. For \( \nu = 0 \), \( \lambda = 0 \) leads to a reflectionless potential [27] and as \( \lambda \) increases the potential takes the form of a double-well potential near the bridge throat. For \( \nu = 1 \), the centrifugal term enhances the barrier near the origin.

The PDM parameter also modifies the number and behavior of the bound states. For \( \lambda_c < \lambda < 0 \), only one bound state located around the origin was found. As \( \lambda \) increases keeping the volcano-shaped potential the width of the bound state also increases. For \( \lambda > 0 \), the PDM parameter breaks the bound state degeneracy leading to two states. Nonetheless, for greater values of \( \lambda \), the double-well symmetry restores the degeneracy. In fact, there are two hybrid states, and these states are degenerate [47]. The probability density function of these states indicates that resonant tunneling is possible. Our results also indicate that if the coupling factor continues to increase, that double potential well
Fig. 8 The bound states and their probability densities for a catenoid with radius $R = 70 \text{Å}$ and $\nu = 0$. The solid black line represents the effective potential for: a $\lambda = -850 \text{Å}^2$, c $\lambda = 0 \text{Å}^2$, e $\lambda = 10^3 \text{Å}^2$ and g $\lambda = 10^5 \text{Å}^2$. The dashed red and blue dotted lines correspond to the first and second bound states and their probability densities, respectively.

Fig. 9 The bound states and their probability densities for a catenoid with radius $R = 70 \text{Å}$ and $\nu = 1$. The solid black line represents the effective potential for: a $\lambda = -4850 \text{Å}^2$, c $\lambda = -3000 \text{Å}^2$, e $\lambda = 10^3 \text{Å}^2$ and g $\lambda = 10^5 \text{Å}^2$. The dashed red and blue dotted lines correspond to the first and second bound states and their probability densities, respectively.

As future developments, we point out the analysis of the transport features of this graphene bridge, as well as the interaction of the confined electrons with electromagnetic fields.

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