Relativistic quantum dynamics on a double cone

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Abstract
In this paper, we study the relativistic quantum problem of a particle constrained to a double cone surface. For this purpose, we build the Dirac equation in a curved space using the tetrads formalism. Two cases are analysed. First, we consider a free particle on the conical surface, and then we add an uniform magnetic field. In the first case, the exact energy spectrum is obtained and its non-relativistic limit compared to previously published results. In the second case, the spectrum is also exactly obtained and a detailed analysis considering all possible combinations of signs of the quantum numbers reveals the occurrence of highly degenerate zero energy modes. The results obtained here can be applied, for instance, in the investigation of the electronic and transport properties of condensed matter systems that can be described by an effective Dirac equation, such as graphene and topological insulators.

Keywords: relativistic quantum dynamics, motion on double cone, Landau levels

(Some figures may appear in colour only in the online journal)
1. Introduction

The dynamics of quantum particles on surfaces is an exciting research area due to its experimental realisation with interfaces, like in the quantum Hall effect [1], or real two-dimensional materials like graphene [2] and its curved versions (nanocones, nanotubes, etc) and topological insulators [3]. Conical surfaces, in particular, are of special interest in the study of quantum phenomena due to the singular curvature they carry [4]. Effectively, they appear in investigations on topological defects in continuum media [5], cosmic strings [6] and even black holes [7]. In recent years, the quantum dynamics of charge carriers in the presence of different topological defects have been investigated in the aforementioned materials, such as dislocations [8, 9] and disclinations [10, 11].

Double conical surfaces have been much less studied. The classical and quantum dynamics of a particle moving on a double cone was presented in [12]. Classically, the apex of the cone works like a filter, allowing only particles with zero angular momentum to pass from one cone to the other, following a straight line. Consequently, any small perturbation in the angular momentum causes a drastic change in the trajectory of the particle, making the rectilinear motion unstable. Traces of instability in the movement are also observed in the quantum regime.

In [13], ab initio calculations were made with carbon double cones. The results show that they have low formation energy and therefore it is expected that they may be obtained experimentally. This possibility motivated us to extend the work of [12] to the relativistic domain, looking specifically at the Dirac equation and its solutions for a particle on the double cone both with and without magnetic field. Since a class of low-dimensional materials [3, 11, 14, 15] have been theoretically described by an effective Dirac equation, the results obtained here may be applied to condensed matter systems as well.

The organisation of the paper is as follows. In section 2 we describe the geometric model for a double cone surface. We explain in this section why the usual coordinate system used for a conical surface with a single nappe is inconvenient for a double cone surface, and build a new coordinate system extending the radial coordinate. Using this reference frame we obtain the solution of the Dirac equation for the free particle on the conical surface in section 3. In section 4, the problem is extended to the case which includes an external uniform magnetic field parallel to the cone axis. There, we obtain the energy spectrum and analyse how the geometry of the surface changes the spectrum. The paper is summarised and concluded in section 5.

2. Geometric approach

Considering the spherical coordinate system, we can build the surface of a cone simply by fixing the angular coordinate $\theta$. In the case of a double cone surface, a drawback comes up when we use this approach. Since a double cone has two nappes, we cannot use the spherical coordinate system with just a fixed value for the angular coordinate $\theta$, since it is necessary two values, one for each nappe. In order to avoid the complications of working with a discrete coordinate (for instance: to establish a metric in this space would be a problem), we extend the radial coordinate domain for the entire set of real numbers, as done in [12]. Accordingly, the bottom nappe corresponds to the negative values of the radial coordinate, but with the same value of $\theta$ as the points on the upper nappe (see figure 1).

The coordinate system used in this article can be described by the following relations [12]:

\begin{align}
  x &= l \sin \theta \cos \phi, \\
  y &= l \sin \theta \sin \phi, \\
  z &= l \cos \theta,
\end{align}

(1)
The equation of the double cone surface in terms of this coordinate system is therefore \( \theta = \text{const} \), whereas in the three–dimensional Cartesian coordinates it is \( x^2 + y^2 = z^2 \tan^2 \theta \). The induced metric of the cone is thus \( g_{\theta\phi} = \sin^2 \theta \), and therefore can assume values only in the \( 0 < \alpha < 1 \) range.

We are interested in investigating the relativistic problem of a particle constrained to a double cone surface in the spirit of the non-relativistic problem studied in [12]. In the following section, we build the Dirac equation for a free particle within the geometric scenario discussed above.

3. Dirac equation of a free particle on a double cone surface

In order to build the Dirac equation in a curved space, one can use the tetrad formalism [16, 17]. This formalism is required in curved space because in this background the spinors must be defined locally. A local reference frame can be built by a non-coordinate basis \( \Theta^a = \epsilon_{a}^\mu(x)dx^\mu \), whose components \( \epsilon_{a}^\mu(x) \) are called tetrads. As notation, we are using Greek indices for coordinates of the curved spacetime, while Latin indices denote the local reference frame of the observers.

We can use the tetrad formalism to relate the metric for the curved space to the flat space metric

\[
\begin{align*}
\text{Figure 1.} \text{ Coordinate system for a double cone surface. With the extension of the radial coordinate domain, a point in the bottom nappe has the same } \theta \text{ coordinate as a point in the upper nappe.}
\end{align*}
\]

\[
g_{\mu\nu}(x) = \epsilon_{\mu}^a(x)\epsilon_{\nu}^b(x)\eta_{ab},
\]
where \( \eta_{ab} = \text{diag}(-c^2, +1, +1) \) is the Minkowski metric tensor. In order to write the Dirac equation for a curved background, we use the tetrads \( e_{\mu}^{\alpha}(x) \) to intermediate some changes in the usual equation. The gamma matrix, \( \gamma^\mu \), will be now defined in terms of the field \( e_{\mu}^{\alpha}(x) \),

\[
\gamma^\mu(x) = e_{\mu}^{\alpha}(x)\gamma^\alpha,
\]

where \( \gamma^\mu = (\gamma^0, \gamma^1, \gamma^2)^T \) and \( \gamma^a = (\gamma^0, \gamma^1, \gamma^2)^T \). The covariant derivative of spinor field is given by \( \nabla_\mu \Psi = \partial_\mu \Psi + \Omega_\mu \Psi \), where the spinorial connection is

\[
\Omega_\mu = \frac{1}{4} \omega_{\mu ab} \Sigma^{ab},
\]

\( \Sigma^{ab} = \frac{1}{2} [\gamma^a, \gamma^b] \) and \( \omega_{\mu ab} \) is a 3–form, known as spin connection. With these elements, we can write the Dirac equation for a curved space as

\[
[i\hbar c \gamma^\mu (\partial_\mu + \Omega_\mu) - mc^2] \Psi = 0.
\]

For a double cone surface, which has the metric (3), the condition (4) allows us to choose the triad

\[
e_{\mu}^{\alpha} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \frac{1}{\alpha l} \end{pmatrix}.
\]

With this triad we determinate the gamma matrices for a double cone surface using the relation (5). We obtain

\[
\gamma^0 = \gamma^1, \\
\gamma^1 = \gamma^0, \\
\gamma^0 = \frac{\gamma^2}{\alpha l}.
\]

Following [18], we write the \( \gamma \) matrices conveniently in terms of the Pauli matrices as

\[
\gamma^0 = \sigma^3, \\
\gamma^0\gamma^1 = \sigma^1, \\
\gamma^0\gamma^2 = s\sigma^2.
\]

where \( s \) is twice the spin value, with \( s = +1 \) for spin up, and \( s = -1 \) for spin down.

The spin connection is obtained from the first Cartan structure equation, given by

\[
d\theta^a + \omega^a_b \wedge \theta^b = 0.
\]

Since \( \omega^a_b = \omega_{\mu ab}dx^\mu \), we get the following non-null spin connection components

\[
\omega_{\mu 21} = -\omega_{\mu 12} = \alpha.
\]

The relation between the spin connection and the spinorial connection is expressed in (6). Using this relation and the result (11), we obtain only one nonnull component for the spinorial connection

\[
\Omega_\phi = \frac{i}{2} \alpha s \sigma^3.
\]
With all these quantities determined for the double cone surface, we can write the resulting Dirac equation as

\[
i \hbar c \left[ \gamma_0 \partial_t + \gamma_1 \partial_x + \gamma_2 \frac{1}{\alpha l} (\partial_\phi - i/2 \alpha \sigma_z) \right] \Psi - mc^2 \Psi = 0.
\] (13)

It is natural to choose as ansatz, solutions like

\[
\Psi(t, l, \phi) = e^{-i\phi/\alpha} e^{\psi_A(t) l} e^{\psi_B(t) l},
\] (14)

where \(E\) and \(J\) are constants of integration and can be interpreted as energy and angular momentum quantum number, respectively. Periodicity in the azimuthal angle \(\phi\) implies that \(J = 0, \pm 1, \pm 2, \pm 3..., j \in \mathbb{Z}\). With the ansatz (14), we write the equation (13) in terms of two coupled differential equations

\[
(E - mc^2)\psi_A = -i\hbar c \left( \partial_t + \frac{1}{2J} \right) \psi_B - \frac{i\hbar c}{\alpha j} \psi_B,
\] (15)

and

\[
(E + mc^2)\psi_B = -i\hbar c \left( \partial_t + \frac{1}{2J} \right) \psi_A + \frac{i\hbar c}{\alpha j} \psi_A,
\] (16)

where \(\psi_A = \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix}\). Uncoupling these equations, we get for \(\psi_A\)

\[
I^2 \partial_t^2 \psi_A + I \partial_t \psi_A + [K^2 l^2 - \nu^2] \psi_A = 0,
\] (17)

where we defined

\[
K^2 = \frac{1}{\hbar^2 c^2} \left( E^2 - m^2 c^4 \right),
\] (18)

\[
\nu = \left( \frac{J}{\alpha} - \frac{s}{2} \right).
\] (19)

The expression (17) is the Bessel equation. We can write the solution for this equation as a combination of Bessel functions of the first kind. We avoid the solution of second kind because it diverges at the origin of the coordinate system. Therefore we get for \(\psi_A\)

\[
\psi_A(Kl) = CJ_\nu(Kl)
\] (20)

where \(C\) is a normalisation constant. The solution for \(\psi_B\) is found substituting (20) in (16). The result after some calculations is

\[
\psi_B(Kl) = \frac{i\hbar c K}{E + mc^2} CJ_{\nu+1}(Kl)
\] (21)

In order to compare our results with the solution of the Schrödinger equation obtained in [12], let us consider the non-relativistic limit of the Dirac equation for the double cone surface. This limit is obtained by defining the non-relativistic energy as the energy measured from \(mc^2\), that is, \(\epsilon = E - mc^2\). In that limit the component \(\psi_A\) is much bigger that \(\psi_B\), so we neglect \(\psi_B\). For \(\psi_A\) we get
which is basically the same equation obtained in [12], except by the spin-orbit term \( \frac{\hbar}{\hat{l}} \) presents in \( \nu \). The Schrödinger equation was obtained in the aforementioned article by using a linear momentum operator modified to become self-adjoint. We do not use this approach in the relativistic case because all the information on the geometry is already incorporated into the Dirac equation through the metric and the spinorial connection. This takes care of the self-adjointness of the operators involved.

As discussed in [12], the dynamics of a particle in a double cone is intimately related to its angular momentum. In the classical approach, using the Hamiltonian formalism, it is shown that the cone apex, that is, the origin of the coordinate system, works like a filter and only particles with zero angular momentum can travel between the two cones. The peculiarity of the zero angular momentum state remains in the quantum regime as pointed out in [12].

4. Dirac equation of a double cone surface in the presence of an uniform magnetic field

We consider now the case of a particle on a double cone surface in the presence of an uniform magnetic field in the direction of the \( z \)-axis, \( \hat{B} = B_0 \hat{z} \), as can be seen in figure (2). The magnetic field is incorporated to the Dirac equation by minimal coupling. So, we have that

\[
P \partial_t \psi_A + i \partial_\nu \psi_A + \left[ \frac{2m e}{\hbar^2} \nu^2 - \nu^2 \right] \psi_A = 0,
\]

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\[
[ih c \gamma^\alpha (\partial_\alpha + \Omega_\alpha) + e Q \gamma^\alpha A_\alpha - mc^2] \Psi = 0,
\]

where \( e \) is the positive unit of charge, taken as usual to be equal to the proton charge and \( Q = \pm 1 \) according to the signal of the charge. In the previous section, we determined the spinorial connection (12), as well as the gamma matrices (10). The only quantity that we have to specify here is the vector potential \( A_\mu \) which we choose in the gauge

\[
\bar{A} = \frac{B_0 |\vec{l}|}{2} \hat{\phi},
\]

where the modulus of \( \vec{l} \) appears here to ensure that the direction of \( \vec{B} \) is preserved after extending the domain of \( l \). Note that, the magnetic field permeates the three-dimensional space and therefore is obtained from the curl of the vector potential in flat space coordinates.
With the results (12) and (24) and defining the field locally, we can write the Dirac equation (23) for the problem of a particle in a double cone surface in the presence of a magnetic field as
\[
\imath\hbar c \left[ \frac{\gamma^0}{c} \partial_t + \gamma^i \partial_i + \frac{\gamma^2}{\alpha l} \partial_\psi + \frac{\gamma^2}{\alpha l} \left( -\frac{i}{2} \alpha \sigma^3 \right) \right] \Psi + eQ\gamma^2 \left( \frac{B_0 |l|}{2} \right) \Psi - mc^2 \Psi = 0.
\] (25)

In order to solve this equation, we choose the ansatz (14) and, taking into account the convention (12), we obtain two coupled differential equations given by
\[
(E - mc^2)\psi_A = -\imath\hbar c \left( \partial_t + \frac{1}{2l} \right) \psi_A - \frac{i \hbar c j s}{\alpha l} \psi_A + \frac{ieQsB_0 |l|}{2} \psi_A.
\] (26)
\[
(E + mc^2)\psi_B = -\imath\hbar c \left( \partial_t + \frac{1}{2l} \right) \psi_B + \frac{i \hbar c j s}{\alpha l} \psi_B - \frac{ieQsB_0 |l|}{2} \psi_A.
\] (27)

To uncouple the above equations and work with a unified solution, we define the quantity
\[
\eta = \frac{|l|}{l} = \begin{cases} +1, & \text{for } l \geq 0, \\ -1, & \text{for } l < 0. \end{cases}
\] (28)

It is important to note that the parameter \( \eta \) is a new quantum number that indicates in which nappe of the double cone the particle is. With this quantity, we can uncouple the differential equations (26) and (27) and obtain for \( \psi_A \)
\[
\frac{d^2}{dt^2} \psi_A + \frac{1}{l} \frac{d}{dl} \psi_A - \frac{1}{l^2} \nu^2 \psi_A + K_{\text{mag}} \psi_A - \left( \frac{eB_0}{2\hbar c} \right)^2 l^2 \psi_A = 0,
\] (29)
where
\[
\nu = \left( \frac{j}{\alpha} - \frac{s}{2} \right),
\] (30)
\[
K_{\text{mag}} = \frac{1}{\hbar^2 c^2} (E^2 - m^2 c^4) + \frac{eQB_0 |l|}{\hbar c} \left( \frac{j}{\alpha} + \frac{s}{2} \right).
\] (31)

In order to simplify the equation (29) we perform the change of variables \( \zeta = \left( \frac{eB_0}{2\hbar c} \right) l^2 \). With this new coordinate, we write
\[
\frac{d^2}{d\zeta^2} \psi_A + \frac{1}{\zeta} \frac{d}{d\zeta} \psi_A - \frac{1}{4\zeta^2} \nu^2 \psi_A + \frac{K'_{\text{mag}}}{\zeta} \psi_A - \frac{1}{4} \psi_A = 0,
\] (32)
where
\[
K'_{\text{mag}} = \frac{\hbar c}{2eB_0} K_{\text{mag}}.
\] (33)

To solve this equation, we look at its asymptotic behaviour in the limits \( l \to \pm \infty \) and \( l \to 0 \). This technique involves the evaluation of the solutions in the asymptotic limits and the proposal of a function which gives the same solution at these limits. By using this approach, we obtain the solution
Replacing the solution (34) into equation (29), we get the following equation
\[ \zeta
\begin{align*}
\psi_A &= e^{-\frac{\zeta}{\alpha}} F(\zeta) \tag{34} \\
\end{align*}
\]
Replacing the solution (34) into equation (29), we get the following equation
\[ \zeta \frac{d^2}{d\zeta^2} F(\zeta) + \left(|\psi| + 1 - \frac{\zeta}{2}\right) \frac{d}{d\zeta} F(\zeta) + \left(K_{mag}' - \frac{|\psi| + 1}{2}\right) F(\zeta) = 0. \tag{35} \]
This is a confluent hypergeometric equation and \( F(\zeta) \) is a confluent hypergeometric function that can be expressed as \( F\left(K_{mag}' - \frac{|\psi| + 1}{2}\right) \). Once found the solution for \( \psi_A \) in (34), the upper component of the spinor \( \Psi \) in (14) is determined. The same procedure can be used to find the lower component \( \psi_B \) (substitute (34) in (27) and use properties of the hypergeometric confluent function). Since we are not interested in the antiparticles, we leave this aside and keep working with \( \psi_A \).

To get physically acceptable solutions, that is, normalisable solutions, we need to truncate the hypergeometric series. This condition leads us to impose that \(-n = \left(-K_{mag}' + \frac{|\psi| + 1}{2}\right)\), where \( n = 0, 1, 2, \ldots \) and \( \left|\frac{\zeta}{\alpha} - \frac{1}{2}\right| \geq 1 \) (see for instance [19]), which excludes the \( j = 0 \) case. As commented in the end of the previous section, \( j = 0 \) is a very peculiar case which deserves detailed investigation by itself. With the above conditions applied to \( \psi_A \) and taking into account that \( \psi_A \) represents the solution for electrons \( (Q = -1) \), we obtain that the energy spectrum is given by
\[ E^2_{(A)} = eB\hbar c \left[ 2n + 1 + \left| \frac{j}{\alpha} - \frac{s}{2} \right| + \eta \left( \frac{j}{\alpha} + \frac{s}{2} \right) \right] + m^2c^4. \tag{36} \]
Note that the orbital angular momentum for the particle on the cone is \( \hbar j/\alpha \) and not \( \hbar j \) as in the flat case. Since the total angular momentum along the \( z \) direction is now \( \hbar j/\alpha + h\pi/2 \) the degeneracy of the energy states is partially broken as compared to the \( \alpha = 1 \) case.

In order to better analyze the spectrum given by equation (36) we refer to table 1 where we list the possible combinations of sign of the relevant quantum numbers. There is an obvious ‘reflection’ symmetry in the table: simultaneous inversion of signs of \((\eta, s, j)\) leave the spectrum unchanged. More importantly, the lowest energy state is a ‘zero mode’ [20] corresponding to the rest energy, \( E = mc^2 \), which occurs when \((\eta, s, j, n) = (+1, -1, < 0, 0) \) or \((\eta, s, j, n) = (-1, +1, > 0, 0) \). The upper (lower) nappe state is infinitely degenerated with respect to all negative (positive) values of the orbital angular momentum \( j/\alpha \). Reversing the magnetic field is the same as exchanging nappes, thus, all values of orbital angular momentum
will admit zero modes either way. This is related to a remarkable property of two-dimensional Dirac massive fermions known as parity anomaly [20] (a parity transformation is realised when the magnetic field is reversed).

It is worthwhile to compare our solution to the relativistic and non-relativistic, spinless case, as studied in similar systems in [21] and [22], respectively. In both cases, it is studied the quantum dynamics of a charged, spinless, particle in the presence of a linear topological defect which is associated to a conic geometry. In both cases, the energy spectrum is obtained and has a dependence on \[ \frac{2n + 1}{\alpha} \left| -\frac{j}{\eta} \right| \] in agreement with our result.

As expected, the energy spectrum given by equation (36) depends on the parameter \( \alpha \), which gives a measure of the opening angle of the conical surface. As discussed earlier, we considered here that this parameter assumes values in the interval \( 0 < \alpha < 1 \), which is the interval where we have a double cone surface. In this interval, we notice that the energy levels in the case of a conical surface are larger than the corresponding ones in the planar case (\( \alpha = 1 \)). It is possible to see the decreasing of the energy due to the parameter \( \alpha \) in figure 3, where we plot the energy as a function of the magnetic field for \( \alpha = 1 \) (figure 3(a)) and \( \alpha = 0.5 \) (figure 3(b)) for a few values of the quantum number \( j \).

5. Concluding remarks

In this work, we studied the quantum relativistic problem of a particle constrained to a double cone surface with and without an external magnetic field. To accomplish this, we used an appropriate coordinate system, since the usual spherical coordinates lead to some complications on the double cone surface. Within this approach, we constructed and exactly solved the Dirac equation for both cases. Taking the non-relativistic limit of the solution in the absence of magnetic field we reproduced the result previously published in [12]. In the problem with a magnetic field, we verify a parity symmetry in the spectrum and the corresponding zero energy modes.
Since the electronic structure of materials like graphene and topological insulators can be described by an effective Dirac equation, it would be interesting to investigate how the magnetic field affects the energy spectrum of a graphene double cone, which could be useful in future applications of graphene-based devices. We expect to address this problem in forthcoming publications.

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