Wave packets in graphene under external fields: Vortices formation

P.E. de Brito a, H.N. Nazareno b,*

a Universidade de Brasília, FUP, Campus Planaltina, 73300-000 Brasília, DF, Brazil
b International Center of Condensed Matter Physics, Universidade de Brasília, P.O. Box 04513, 70910-900 Brasília, DF, Brazil

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ABSTRACT
In this work we analyzed the time propagation of wave packets on a sheet of graphene under the action of external magnetic and electric fields in the Hall configuration. The treatment given in this work to the problem of particle propagation in graphene is based on the tight-binding model, not requiring to consider the linear approximation of the band structure around point \( K \) in the Brillouin zone. So, our calculation is able to describe the behavior of the particle in more general cases, not only the case of low lying excited states, the so-called massless Dirac electrons. Evaluating the time evolution of the wave function we assume as an initial state a Gaussian with a given velocity. We have considered the symmetric gauge for the vector potential. For specific cases one is able to show a very interesting effect such as the apparition of vortices, i.e., the initial wave is split into components each one of these forming vortices that remain stationaries as time goes. Moreover, for a packet with a wave vector near point \( K \) in the Brillouin zone, one is able to show the presence of the effect of zitterbewegung, that is, a trembling motion of the centroid of the wave packet. The inclusion of a dc electric field in the plane of the graphene lattice displaces the vortices in a direction perpendicular to the field.

1. Introduction

In this work we analyze the wave packet propagation in the 2D graphene lattice under external fields along the tight-binding model. Graphene consists of a one-atom thick sheet of carbon atoms arranged in a planar honeycomb lattice which was first fabricated in 2004 [1]. Since its successful fabrication intense research activity both theoretical and experimental is conducted in several laboratories in the world. The structure consists of a hexagonal lattice with two atoms per unit cell of lattice parameter \( a = 2.49 \, \text{Å} \), while the nearest neighbors carbon–carbon distance is \( a_{C-C} = 1.44 \, \text{Å} \). Recently an excellent review appears on the electronic properties of graphene that includes an extended bibliography [2]. Andrey Chaves et al. in a recent paper [3] have reported results on wave packet propagation in strained graphene obtained along the tight-binding model and the continuous (Dirac) model. Both approaches give qualitatively similar results as long as the wave vector of the packet is close to the Dirac points, obviously this is so because the Dirac continuous model is valid in such a case. In Chapter 22 of the recently published book [4], Maksimova et al. presented a well detailed study of wave packets dynamics in graphene, by considering the continuous Dirac model. They have discussed the way the pseudospin polarization of the wave packet determines its time evolution.

In the present work the inclusion of the magnetic field was taken into account by means of the Peierls substitution [5]. We have solved the time dependent Schrodinger equation by assuming as an initial condition a Gaussian wave packet with a given velocity. Following, we have obtained the trajectories of the centroids as well as the time evolution of the mean-square displacement (MSD) and the participation function [6]. We observe the successive splitting and reconstruction of the wave function into two or more components, that is, vortices formation as a result of the joint effect of the crystal potential and the magnetic field. This remarkable effect was reported by us for the square lattice [7]. We explain below the reason for the vortices formation. We study the trajectories in reciprocal space, since, by rotating them by \( \pi/2 \) we obtain the corresponding ones in real space. The rotating currents predicted here could be detected experimentally by measuring the fluctuating magnetic field produced by them, as well as through imaging experiment that could detect electron trajectories [8,9]. Note that some theoretical predictions in physics came earlier than their experimental verification; as an example of this, the Bloch oscillations [10] predicted in the early days of quantum mechanics were measured several decades later [11], to say nothing of the phenomenon of Bose–Einstein condensation, experimentally verified almost a century after its proposal [12,13]. We also obtain the trembling motion (zitterbewegung) of the centroid of the wave function.
As for the inclusion of a dc electric field, the propagating wave packet presents a complex behavior, at the same time one notes that it propagates in a direction perpendicular to the applied field, as it is in the case of a classical particle subject to the same configuration of the external fields [14]. We would like to remark that our approach is not based on the linear approximation for the energy of the excited electrons, but through the present treatment one is able to consider a more general situation.

In the next section we present the tight-binding Hamiltonian and the method of calculation used to integrate the time dependent Schrödinger equation, while the magnetic field is introduced through the Peierls substitution, while the initial state considered is a Gaussian packet. Next we describe the phenomenon of vortices formation and explain why and when this remarkable effect occurs. After that, the trembling motion (zitterbewegung) is analyzed. It is shown that its apparition happens when the wave vector of the Gaussian is at, or close to, one of the Dirac K points. In the next section the effect of the inclusion of an in-plane dc electric field is presented, showing that the wave packet displaces in a direction perpendicular to the applied field. Finally we summarize the results obtained.

For some figures we have produced short films that they can add to reader’s understanding and present results in attractive ways that go beyond what can be presented in the print version. These films are shown at the web page: http://www.pedebruito.unb.br/index.php?option=com_content&view=article&id=57:graphene&catid=34:tqsd&Itemid=59.

2. The model

The unit cell of the honeycomb lattice has basis vectors: \( \vec{a}_1 = a(\sqrt{3}/2 \hat{y} + 1/2 \hat{x}) \), \( \vec{a}_2 = a(\sqrt{3}/2 \hat{y} - 1/2 \hat{x}) \), where \( a_{\text{c.-c.}} = a/\sqrt{3} \) being the nearest neighbors distance. It is useful to consider the change of basis between the orthogonal basis to the hexagonal one: \( \vec{r} = x \hat{x} + y \hat{y} = z_1 \vec{a}_1 + z_2 \vec{a}_2 \). Note that the variables \( z_1 \) are dimensionless.

The Hamiltonian of the tight-binding model taking into account hopping between the nearest neighbors is

\[
\hat{H} = -W \sum_{n,m} (\hat{b}_{n,m}^\dagger \hat{a}_{n,m} + \hat{b}_{n,m} \hat{a}_{n,m}^\dagger + \hat{b}_{n-1,m}^\dagger \hat{a}_{n,m} + \hat{b}_{n,m} \hat{a}_{n,m-1}^\dagger + \text{c.c.})
\]  

where \( \hat{b}_{n,m} (\hat{a}_{n,m}) \) is the creation (annihilation) operator associated with atom B at the unit cell at site \((n,m)\) in the lattice, while \( \hat{a}_{n,m} (\hat{a}_{n,m}^\dagger) \) is an annihilation (creation) operator for atom A at lattice site \((n,m)\) and \( W \) is the hopping term. We denote with letters A and B the atoms in the two non-equivalent positions in the unit cell. In the honeycomb lattice the nearest neighbors of an A atom are three B atoms, and reciprocally.

We have omitted in the Hamiltonian the term \( \sum_{n,m} \epsilon_{n,m} (\hat{a}_{n,m}^\dagger \hat{b}_{n,m} + \hat{b}_{n,m}^\dagger \hat{a}_{n,m}) \), where the \( \epsilon_{n,m} \) are the on-site energies, which can be taken as zero in a perfect crystal.

We need to solve the time dependent Schrödinger equation in order to obtain the time evolution of wave packets:

\[
\frac{i\hbar}{\partial t} |\Psi\rangle = \hat{H} |\Psi\rangle
\]  

We expand the wave function in the Wannier basis:

\[
|\Psi\rangle = \sum_{n,m} g_{A,n,m} |A,n,m\rangle + g_{B,n,m} |B,n,m\rangle
\]  

We perform a Fourier transform of the Wannier states:

\[
|A,\vec{k}\rangle = \frac{1}{\sqrt{N}} \sum_{n,m} (e^{i \vec{k} \cdot \vec{r}_{n,m}}) |A,n,m\rangle
\]  

and the same for B atoms. \( N \) denotes the number of unit cells. The atom positions in the lattice are defined through the following:

\[
\vec{r}_{A,n,m} = m \vec{a}_1 + n \vec{a}_2 + \delta \vec{a}_c \hat{i} \quad \text{with} \quad \delta = 0(1) \quad \text{for atom A(B)}
\]

Consequently, we obtain for the amplitudes:

\[
g_{A}(\vec{k}) = \frac{1}{\sqrt{N}} \sum_{n,m} (e^{i \vec{k} \cdot \vec{r}_{n,m}}) g_{A,n,m}
\]

\[
g_{B}(\vec{k}) = \frac{1}{\sqrt{N}} \sum_{n,m} (e^{i \vec{k} \cdot \vec{r}_{n,m}}) g_{B,n,m}
\]

It is easy to see that by using these expressions one obtains the equation of motion in the matrix form

\[
\frac{i \hbar}{\partial t} \begin{pmatrix} g_{A}(\vec{k}) \\ g_{B}(\vec{k}) \end{pmatrix} = \begin{pmatrix} 0 & f(\vec{k}) \\ f^*(\vec{k}) & 0 \end{pmatrix} \begin{pmatrix} g_{A}(\vec{k}) \\ g_{B}(\vec{k}) \end{pmatrix}
\]

where

\[
f(\vec{k}) = e^{i \vec{k} \cdot (\vec{a}_1 + \vec{a}_2)/3} + e^{i \vec{k} \cdot (\vec{a}_1 - 2\vec{a}_2)/3} + e^{i \vec{k} \cdot (\vec{a}_2 - 2\vec{a}_1)/3}
\]

If one considers the stationary Schrödinger equation instead, we obtain the band structure already reported by Wallace [15] some decades ago

\[
i\epsilon(\vec{k}) = \pm \sqrt{f(\vec{k})^2}
\]

It is well known that for the wave vector \( \vec{k} \) near the point \( \vec{K} = (0, 4\sqrt{3}/3 \pi/a) \) in the Brillouin zone (see Fig. 1), the energy goes linear with wave vector, which explains the name of massless Dirac electrons given to those carriers, at the same time a point \( \vec{K} \) in the Brillouin zone is called a Dirac point.

As before, we consider the vector potential as given in the symmetric gauge

\[
\vec{A} = \frac{B}{2} (-y \hat{x} + x \hat{y}) = \frac{\phi}{2} (-z_2 \vec{b}_1 + z_1 \vec{b}_2)
\]

where \( \vec{b}_1 \) and \( \vec{b}_2 \) are the basis vectors in reciprocal space.

At this point we incorporate the magnetic field through the Peierls substitution, namely we transform the wave vector \( \vec{k} \) into

![Fig. 1. The Brillouin zone and the lines of constant energy. The arrows indicate the trajectories in reciprocal space.](image-url)
an operator
\( \hat{\mathbf{k}} \rightarrow -i \left( \frac{\hat{b}_1}{2\pi} + \frac{\hat{b}_2}{2\pi} \right) - \pi z(-z_2 \hat{b}_1 + z_1 \hat{b}_2) \)
(6)

where \( a = \Phi / \Phi_0 \) is the ratio between the flux through the unit cell \( B(a^2 \sqrt{3}/2) \), to the quantum of flux \( \Phi_0 = h c / e \), and \( \hat{c}_1 = \hat{c} / \hat{z} \).

We would like to remark that the approach followed in this work does not consider the linear approximation usually assumed while treating the graphene electrons. By using the Peierls substitution given by the last expression in Eq. (4), one is able to obtain for the time evolution of the Wannier amplitudes the set of equations:

\[
\begin{align*}
\text{i} \hbar g_{A,n,m} &= -W(e^{i\pi(n-m)/3})g_{B,n,m} + e^{i\pi(n+2m)/3}g_{B,n-1,m} + e^{i\pi(n+2m)/3}g_{B,n-1,m-1} \\
\text{i} \hbar g_{B,n,m} &= -W(e^{-i\pi(n-m)/3})g_{A,n,m} + e^{-i\pi(n+2m)/3}g_{A,n+1,m} + e^{-i\pi(n+2m)/3}g_{A,n+1,m-1}
\end{align*}
\]

(7)

(8)

We would like to stress that these last equations are our principal result.

We have used the Runge–Kutta method of fourth order in order to solve the time-dependent Schrödinger equation, we chose as an initial condition a Gaussian wave packet with a certain width and a given velocity \( \Psi(0) = e^{i \mathbf{k} \cdot \mathbf{r}} \frac{1}{\sqrt{\pi}} e^{-(x-x_0)^2 + (y-y_0)^2}/2\sigma^2 \)
(9)

This choice is based on the assumption that the injected electron is not extremely localized. To avoid boundary effects we chose a lattice of 40,000 sites. To be specific we consider \( k = \pi a / 40 \), for a given wave vector \( k \) is in units of \( \pi / a \). We show results for \( \sigma = 2 \). The results presented in this paper along the tight-binding model should be comparable with that obtained within the treatment of Dirac massless electrons near point \( \mathbf{K} \), for a \( (1/2) \) initial pseudo-spinor. After solving the set of equations we evaluate the following:

(i) the mean-square displacement (MSD)

\[
\langle r^2 \rangle = \sum_{n,m,0} |g_{n,m,0}(t)|^2 a^2(n^2 + m^2 + n \cdot m)
\]

(10)

(ii) the trajectory of the centroid of the wave packet

\[
\begin{align*}
\langle x(t) \rangle &= \sum_{n,m,0} x |g_{n,m,0}(t)|^2 \\
\langle y(t) \rangle &= \sum_{n,m,0} y |g_{n,m,0}(t)|^2
\end{align*}
\]

(11)

(12)

where in the discrete coordinate system

\[
\begin{align*}
x &= \left( \frac{\sqrt{3}}{2} (n + m) + \frac{\delta}{2} \right) a \\
y &= \left( \frac{m - n}{2} \right) a
\end{align*}
\]

for \( \delta = 0(1) \) for atom \( = A(B) \)

(iii) the participation function [6]

\[
P(t) = \left[ \sum_{n,m,0} |g_{n,m,0}(t)|^2 \right]^{-1}
\]

(13)

which gives the number of sites that participate in the wave packet at time \( t \).

3. Vortex formation

In this section we describe the interesting behavior observed during the time evolution of the wave function under the combined effect of the lattice and a magnetic field. As it is well described in solid state books, the quasimomentum satisfies the Lorentz equation of motion for a particle in the presence of a magnetic field, where one takes the group velocity \( \mathbf{v} = (1/\hbar)\mathbf{k}/i\mathbf{k} \) which in turn determines that the wave vector moves along the lines of constant energy [16]. As for the trajectories in real space, they are obtained by rotation by \( \pi / 2 \). We started with a Gaussian packet with a given momentum, but due to the structure of it we have a dispersion in \( k \), which implies that several wave vectors will participate in the evolution of the wave function. This plays an important role as long as the wave vector lies around regions in the Brillouin zone (BZ) where the trajectories circulate in different senses. In Fig. 1 we show the lines of constant energy where the arrows signal the orbit in reciprocal space described by the wave vector.

We see that for \( k \) near the center of the BZ, trajectories are close to circular, nothing new so far. That is the case, we show in Fig. 2 the centroid trajectory describing a circle for \( k = (0,0,2) \), that is near the center of the BZ, behavior similar to a classical particle under the action of a magnetic field. Note that the units of \( k \) are \( \pi / a \). In Fig. 2 we also show the time evolution of the MSD and participation function, both functions present an oscillatory behavior associated with the circular trajectory of the centroid.

The novelty comes in one considers, for example, \( k \) at the point \( \mathbf{M}’(k = (0,1)) \), that is, lying in the boundary between hexagonal and triangular trajectories; the wave splits into two, part of the wave describes a trajectory in the clockwise sense and the other part in the opposite sense, the resulting movements consist in the presence of a vortex and an antivortex. The hexagonal trajectory is larger than the triangular one taking more time to complete the orbit. See Fig. 3 where the wave at times \( t = 50 \) and \( t = 100 \) is shown. One notes that for \( t = 50 \) the hexagonal orbit is still not complete, while at \( t = 100 \) the orbit is completed. It is also shown that the time evolution of the MSD and participation function, once the greater orbit is completed one observes a saturation in both functions.

A more complex situation occurs when one takes \( k \) at point \( \mathbf{M}’(k = (2/3,0)) \), that is, at the border of four different regions in reciprocal space. As can be seen in Fig. 4, in this case one has two triangular and two hexagonal orbits along perpendicular directions. One notices the formation of four vortices associated with each of the regions. In Fig. 4 we show the wave packet at four times: \( t = 30, 40, 50 \) and 70, where one can see the packet as it evolves in time. As can be inferred from the figures the different vortices remain localized in a definite region of the lattice.

The energy difference between the one associated to an electron at point \( \mathbf{M}’(M) \) and the Fermi level at point \( \mathbf{K} \) is 2.7 eV. Therefore, this being the amount of energy required to put an electron in the conduction band. In this case the linear approximation breaks down since we are far from the Dirac point \( \mathbf{K} \). This is one of the reasons why we have used the tight-binding model for the present problem.

We have performed several calculations in order to analyze the influence of the dispersion of the Gaussian on the time evolution of the wave packet. The results obtained indicate that for a given \( k \) the centroid trajectories are the same for the different dispersions considered, i.e., the centroid orbits are invariant under a change in the dispersion of the initial wave packet. Wave packets of different extensions produce identical
centroid orbits, while the more extended the initial packet the more rigid it is. This result is in agreement with the one obtained by us in the case of a wave propagating in free space and subject to a magnetic field [17].

4. Trembling motion (zitterbewegung)

Now, taking the wave vector of the Gaussian packet at, and around the K point, we observe a localized wave function, while...
the centroid describes an erratic trajectory around the starting position, that is, we are in the presence of a trembling motion performed by the centroid. We have analyzed the wave propagation associated with three different wave vectors: \( \mathbf{k} = (0, 1.27) \), (0, 4/3) and (0, 1.39). In Fig. 5a–c we show the MSD, participation function, and the centroid trajectories in the \( x-y \) plane, respectively, for the three cases. In all the three cases the behavior is the same, a well localized wave packet that is clearly seen through the MSD and participation function, together with the trajectory of the centroid in a limited region of the lattice; we have a
We consider now the inclusion of an in-plane dc electric field in the equation of motion for the Wannier amplitudes. To take into account the electric field in the calculations, we include in the equations of motion the diagonal terms $\varepsilon \mathbf{E} \cdot \mathbf{R}_{n,m,\alpha} \delta_{n,m,\alpha}$. These diagonal terms become:

$$ea \left[ (n+m) \frac{\sqrt{3}}{2} E_x + (m-n) \frac{1}{2} E_y \right] \delta_{n,m,\alpha}$$

(14)

As a general trend, we observe that the packet will propagate in a more complex way, but always in a direction perpendicular to the electric field, as it was shown previously [21]. This behavior is also present in the classical treatment of the problem [14]. From the viewpoint of quantum mechanics, we understand this behavior since the electric field breaks the degeneracy of the on-site energies along the direction of the applied field, therefore inhibiting hopping between these sites. We have made a simulation considering an electric field along the x-direction $E = (0,3,0)$ and with $\mathbf{k} = (0,4/3)$ that is at point K. We illustrate this in Fig. 6 where one notes a displacement of the packet along the y-direction at the same time that it performs an oscillatory movement in the perpendicular direction. We show the wave packet at different times as well as the centroid trajectory in the $(x,y)$ plane and the MSD as function of time. Another case in study was the following: field now in the y-direction $E = (0,0.3)$ and $\mathbf{k} = (0,2,0)$, that is near the I' point in the BZ. As before the displacement is perpendicular to the field. In Fig. 7 we show the wave at different times as well as the centroid trajectory and MSD. In both cases, one notes that the inclusion of a dc field displaces the wave packets in a perpendicular direction, at the same time they perform oscillatory movements along the field direction, resembling the Bloch oscillations. The composite movement results in a reptilian displacement of the wave packets.

5. Effect of a dc electric field

We consider now the inclusion of an in-plane dc electric field in the equation of motion for the Wannier amplitudes. To take into account the electric field in the calculations, we include in the equations of motion the diagonal terms $\varepsilon \mathbf{E} \cdot \mathbf{R}_{n,m,\alpha} \delta_{n,m,\alpha}$. These diagonal terms become:

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6. Conclusions

In this work we have explored the kind of propagation that a Gaussian wave packet with a given velocity performs, when injected in a graphene sample subject to external magnetic and electric fields in the Hall configuration. Using the Runge-Kutta method of fourth order, we have integrated the equations of motion in the Wannier representation. As for the magnetic field, one is able to observe the split of the injected wave packet causing the formation of vortices, provided the wave vector associated with the Gaussian lays around certain points of the Brillouin zone. These vortices remain stationary...
as long as there is not an electric field applied in the sample. The nature of the vortices depends naturally on the specific wave vector of the initial packet. We illustrate the cases of the formation of two and four vortices. For wave vector at, or around the $K$ point, we have shown the apparition of a trembling motion of the wave packet centroid, the more so, the closer is the $k$ to the Dirac point. The inclusion of an in-plane dc electric field has the effect of moving the vortices in a direction perpendicular to the field. Beside its displacement, the wave is split and reconstructed as time goes.

To have a better understanding of the propagation nature of wave packets in graphene, we have produced short films that illustrate the effect, among other thing, of vortices formation and Bloch oscillations. In the figure captions we made reference to each of the films.

References


