Scattering of massless Dirac fermions in circular p-n junctions with and without magnetic field

Neetu Agrawal (Garg)¹, Sankalpa Ghosh² and Manish Sharma³

1 Centre for Applied Research in Electronics, Indian Institute of Technology Delhi, New Delhi-110016, India
2 Department of Physics, Indian Institute of Technology Delhi, New Delhi-110016, India
3 Atrenta India Pvt. Ltd., A-12, Sector 2, NOIDA, UP 201303, India

E-mail: sankalpa@physics.iitd.ac.in

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Abstract
In the absence of a magnetic field, a scattered wavefunction inside a circular p-n junction in graphene exhibits an interference pattern with its high intensity maximum located around the caustics. We investigate the wavefunctions in the presence of a uniform magnetic field outside the circular region to show how the loci of the high intensity region changes by forming a Landau-level structure outside the circular region and a central high intensity region inside the circular p-n junction due to the strong reflection of massless Dirac fermions by the outside magnetic field. We conclude by suggesting experimental ways to detect such changes in pattern due to the effect of the magnetic field.

Keywords: circular p-n junction, magnetic dot, caustics, graphene, Landau levels

1. Introduction
Electron transport in graphene with an applied split gate voltage is akin to light propagating through a metamaterial with negative refractive index. This analogue can be used to understand the focusing of an electric current by a single p-n junction in graphene and was theoretically predicted in a seminal work by Cheianov et al [1]. It was shown that for the case of a symmetric n-p junction when \( k_n = k_p \), where \( k_n \) (\( k_p \)) is the wave number in the n (p) region, the n-p junction provides perfect focusing of the emitted electrons on the p-side. However, for the case of asymmetric n-p junctions when \( k_n \neq k_p \), the sharp focus transforms into a pair of caustics, which in the language of optics corresponds to an envelope of a family of rays (wavevectors for the electrons) in which the density of rays is singular.

The cusp-shaped patterns of light reflecting on the inside of a coffee cup, the patterns of bright lines observed on the bottom of a swimming pool and the common rainbow are some prime examples of this phenomenon occurring in nature. Since the rays in geometrical optics are analogous to classical trajectories of electrons, the concept of caustics has already been taken forward to atomic [2] and nuclear scattering experiments [3] where a phenomenon analogous to a rainbow has been observed. Observation of caustics in the trajectories of cold atoms in a linear magnetic potential [4] have also been reported. Such focusing and caustic formation of charge carriers also arises in circular n-p junctions of monolayer graphene [5]. The scattered wavefunction of an incoming plane wave of electrons due to a circular symmetric step-like potential shows an interference pattern which resembles that of ‘cup caustics’ [6] (see figure 1), with the high intensity maximum located around caustics that can be calculated from Snell’s law with negative refractive index [5]. Complex caustic patterns have also been demonstrated in the presence of Rashba spin–orbit interaction in the circular gated or doping-controlled region in graphene [7]. This was shown to result in selective focusing of different spins, and the possible direct measurement of the Rashba coupling strength in scanning-probe experiments.

Whereas the focusing and caustic formation can create a region of high intensity for electrons in a circular p-n junction, one may ask what will happen to the probability distribution in presence of a suitable magnetic field. Such a
query is motivated by the fact that magnetic barriers of different geometries are known to confine the charge carriers in monolayer graphene that are massless Dirac fermions \([8–10]\). Whereas the scattering problem of such massless Dirac fermions in the circular potential barrier and the resulting caustic formation is studied in detail for monolayer \([5]\) and bilayer \([11, 12]\) graphene, the fate of such optical analogies for the case of magnetic barriers is yet to be analyzed. This is due to the localized nature of solutions which occur in the presence of magnetic field.

However, it may be pointed out that interesting features, such as the periodic spatial modulation of current injected from a point source near a p-n junction in graphene in the presence of a uniform magnetic field, have been predicted and shown to originate from the caustic bunching of skipping/snake orbits \([13, 14]\). In the present work, we investigate the wavefunction patterns in the presence of a graphene magnetic dot. The geometry corresponds to the magnetic field which is constant except within a disc where it vanishes. One of the ways in which such an inhomogeneous magnetic field can be experimentally realized is by depositing a superconducting disc on the top of the graphene sheet. When a homogenous magnetic field is applied perpendicularly, the magnetic flux lines are expelled from the superconducting disc due to the Meissner effect, which results in the proposed inhomogenous magnetic field profile. Other methods of creating such an inhomogeneous magnetic field for two-dimensional electronic systems were recently reviewed in \([10]\).

For the case of a non-relativistic two-dimensional electron gas (2DEG) system, such a magnetic field profile was discussed in \([15–17]\) to study the bound states and analyze the optical absorption spectrum \([15]\) of such a system. The energy spectrum for a magnetic dot in graphene has been discussed in detail in \([8]\). The spectrum shows a set of bound states below the lowest bulk Landau level which can be employed to design and control an artificial atom in a graphene nanostructure. This energy spectrum is different from the energy spectrum for Schrödinger electrons in terms of the energies of the bound states, which are a consequence of the different energies of the corresponding Landau levels. It may however be noted that in \([18]\) a complementary configuration of the magnetic field was considered, where the magnetic field is nonzero only in a finite, circular disc-like region of space, and vanishes outside that region. In the same work it was shown that in such a situation true bound state solutions are not possible and only quasi-bound states can be defined. Thus this configuration provides a very different spectrum as compared to the case under consideration in this paper. Given this significant change in the energy spectrum in the presence of the proposed magnetic field profile, we investigate what will happen to the caustic formation of the Dirac electron wave functions of monolayer graphene in circular p-n junctions.

The paper is organized as follows. We begin by understanding the scattering of the incident plane wave of ballistic electrons on a circular potential step and obtain the interference pattern which resembles ‘cup caustics’ that can be described in terms of geometrical optics. In the next section, for the case of a magnetic dot, we consider the electrons to be incident (in all directions) from inside the dot which is the field-free region, and analyze the interference patterns. The results and discussion as well as the description in terms of a classical treatment is then presented in the section thereafter.

2. Theory

2.1 Circular n-p junction

We consider charge carriers in graphene in the presence of a circular gate potential

\[
V(\mathbf{r}) = V_0 \Theta(R - r)
\]

(1)

In the absence of intervalley scattering, the low-energy dynamics for graphene charge carriers is described by the following Dirac-like Hamiltonian in-plane polar co-ordinates

\[
\mathbf{H} = -\frac{i e}{\hbar v_F} \begin{pmatrix}
0 & e^{-i\phi} \left( \frac{\partial}{\partial r} - \frac{i}{r} \frac{\partial}{\partial \phi} \right)

\end{pmatrix} + V(\mathbf{r})
\]

(2)
For a rotationally symmetric scalar potential form, such as the one chosen here, the pseudo-angular momentum operator $J_z = -i\hbar \partial_{\phi} + \hbar \sigma_z/2$ commutes with the Hamiltonian.

$$[J_z, H] = 0 \quad (3)$$

For this reason the wavefunction solutions can be constructed in the following form [19]:

$$\Psi_j(r, \phi) = e^{i \phi} \Psi_j(r) \quad (4)$$

$$\Psi_z(r, \phi) = e^{i (l+1) \phi} \Psi_z(r) \quad (5)$$

where $l \in \mathbb{Z} = \{ \ldots, -1, 0, 1, \ldots \}$ is the pseudo-angular momentum which is a conserved quantity here. On substituting equation (5) to solve for $H \Psi = EV$ in equation (2), we obtain the following set of coupled equations:

$$(\frac{\partial}{\partial r} - i \frac{l}{r}) \Psi_j(r) = i \frac{E - V}{\hbar V} \Psi_z(r) \quad (6)$$

$$(\frac{\partial}{\partial r} + i \frac{l + 1}{r}) \Psi_z(r) = i \frac{E - V}{\hbar V} \Psi_j(r). \quad (7)$$

On decoupling the above set of equations we obtain

$$(kr)^2 \frac{\partial^2 \Psi_j}{\partial (kr)^2} + (kr) \frac{\partial \Psi_j}{\partial (kr)} + [(kr)^2 - l^2] \Psi_j = 0. \quad (8)$$

$l$ being an integer, the general solution for the above equation is given as

$$\Psi_j(r) = c_1 J_l(kr) + c_2 Y_l(kr).$$

However, since $Y_l(kr)$ diverges as $r \to 0$ one can instead use Hankel's functions

$$H_{l}^{(1,2)}(kr) = J_l(kr) \pm i Y_l(kr)$$

with the asymptotics at $kr \gg 1$

$$H_{l}^{(1,2)}(kr) \approx \sqrt{\frac{2}{\pi kr}} \exp \left\{ \pm i \left[ kr + \frac{l\pi}{2} - \frac{\pi}{4} \right] \right\} \quad (9)$$

Thus, the function $H_l^{(1)}$ describes the scattering wave and $H_l^{(2)}$ describes the wave falling at the centre. By expanding the incident plane wave (taken parallel to the $\phi = 0$ axis) in terms of eigenfunctions in polar coordinates, the net wavefunction at $r > R$ can be given as [19]

$$\Psi_{j \to R} = \sum_{l=\infty}^{\infty} \left\{ \frac{iJ_l(qr) + b_l H_{l}^{(1)}(kr)}{s^2 + 1} J_{l+1}(kr) + b_{l+1} H_{l+1}^{(1)}(kr) \right\} e^{i (l+1) \phi} \quad (10)$$

where $s = \text{sgn}(E)$, $k = \frac{E}{\hbar V}$ and the terms proportional to the Bessel (Hankel) functions describe incident (scattering) waves. At $r < R$, $k$ should be replaced by

$$q = \frac{|E - V|}{\hbar V} \quad (11)$$

and only the Bessel functions $J_{l}(qr)$ are allowed (otherwise, the solution will not be normalizable, due to the divergence of $Y_l(z)$ at $z \to 0$). Then

$$\Psi_{l < R} = \sum_{l=\infty}^{\infty} a_l \left\{ \frac{iJ_l(qr) e^{i\phi}}{s^2 + 1} J_{l+1}(qr) e^{i(l+1)\phi} \right\} \quad (12)$$

Here $s' = \text{sgn}(E - V_0)$ and the complex factors $b_l$ and $a_l$ in equations (10) and (12) are scattering coefficients. Upon matching the wavefunctions at the boundary $r = R$, we obtain

$$b_l = \frac{J_l(qR) J_{l+1}(kR) - (s'/s) J_{l+1}(qR) J_l(kR)}{(s'/s) H_{l}^{(1)}(kR) J_{l+1}(qR) - J_l(qR) H_{l+1}^{(1)}(kR)} \quad (13)$$

$$a_l = \frac{H_{l+1}^{(1)}(kR) J_{l+1}(qR) - (s'/s) J_{l+1}(qR) H_{l+1}^{(1)}(kR)}{H_{l}^{(1)}(kR) J_l(qR) - (s'/s) J_l(qR) H_{l}^{(1)}(kR)} \quad (14)$$

Using the above expressions (10), (12), (13) and (14) we evaluate the probability density which can be plotted as shown in figure 1(c). For the scattering of an incident plane wave on a circular p-n junction, the region of high probability density can be seen to make a certain pattern which is similar to that of a ‘cup caustic’ (see figure 1).

In the following section we evaluate analytically the equations governing these caustic patterns, which is in accordance with an analogy with geometrical optics.

2.2 Recapitulating caustic formation in the n-p junction

In accordance with an analogy with geometrical optics, a ray incident at an impact parameter $b = R \sin \alpha$ is refracted at an angle $\beta = \sin^{-1}\left(\frac{\sin \alpha}{|b|}\right)$. Incident rays with different impact parameters ($-R < b < R$) form a family of rays inside the circle. If a family of rays (for different impact parameters) is traced, they form a curved envelope. This envelope is the caustic. This can be found from the condition that for a ray incident at an impact parameter $b = R \sin \alpha$, any point $(x_c, y_c)$ lying on the refracted ray, at a ray length $w$, with the mapping $(w, \alpha) \to (x_c, y_c)$ is singular. Mathematically, this is given by the condition that

$$\text{det } \mathcal{J} = 0 \quad (15)$$

For a ray undergoing single reflection from the circular n-p junction,

$$\begin{align*}
    x_c &= -R \cos \alpha + w \cos(\alpha + \beta) \\
    y_c &= R \sin \alpha - w \sin(\alpha + \beta)
\end{align*} \quad (16)$$

so the condition (15) determines

$$w = \frac{R \cos \beta}{1 + \beta'}$$

The envelop as determined with this mapping is plotted (magenta curve) in figure 1(b). For a ray undergoing $p - 1$ internal reflections from the n-p junction, the envelope is determined as [5],

$$\begin{align*}
    \frac{R}{R'} &= (1 - \mu)^p \left[ \left( \frac{-\cos \zeta}{\sin \zeta} + \cos \beta + 2(2p - 1)\beta' \right) \left( \frac{\cos (\zeta + \beta)}{\sin (\zeta + \beta)} \right) \right] \quad (17)
\end{align*}$$
where
\[ \zeta = \alpha + 2(p - 1)j \beta' = \frac{\cos \alpha}{\sqrt{r^2 - \sin^2 \alpha}} \]  

(18)

This is a parametric curve for caustics and is plotted in figure 1(b) for \( p = 1 \) (magenta curve), 2 (green curve), 3 (blue curve). In both cases, we see that the caustic pattern formed from the wavefunction probability distribution obtained using a full quantum mechanical calculation inside the junction agrees very well with that obtained from Snell’s law with negative refractive index. In the next section we investigate such probability density patterns for the case of a magnetic dot.

2.3 Magnetic dot

In this section we investigate the effect of a magnetic field \( \mathbf{B} = B_0 \partial_r (r - R) \) on the scattering pattern in an n-p junction. We begin by calculating the wavefunctions in the presence of a magnetic dot profile as mentioned above. For a radially symmetric magnetic field, adopting the symmetric gauge, the radial and azimuthal components of the vector potential are

\[ A_r(r) = 0; \quad A_\phi(r) = \frac{r^2 - R^2}{2r} \Theta(r - R) \]  

(19)

Then, upon solving for \( H\Psi = E\Psi \) for the Hamiltonian

\[
\begin{bmatrix}
0 & e^{-i\frac{d}{dr} - \frac{1}{r} \frac{d}{d\phi} + A_i - iA_\phi} \\
\exp(-i\frac{d}{dr} + \frac{1}{r} \frac{d}{d\phi} + A_i + iA_\phi) & 0
\end{bmatrix}
\]

the solutions inside the dot are obtained as Bessel’s functions while outside the dot the solutions can be written in terms of confluent hypergeometric solutions. This is shown in detail below. As explained in the previous section, the eigenstates of the above-written Hamiltonian are classified by

\[ \Psi_j(r, \phi) = \begin{cases} 
\Phi_j(r) e^{i(j - 1/2)\phi} \\
\chi_j(r) e^{i(j + 1/2)\phi} 
\end{cases} \]  

(20)

On substituting for \( \Psi_j(r, \phi) \) in \( H\Psi = E\Psi \), we obtain two coupled equations:

\[
\begin{align*}
\frac{d}{dr} + \left( j + \frac{1}{2} - \frac{1}{r} \frac{d}{d\phi} + A_i + iA_\phi \right) \chi_j &= \frac{E}{\hbar v_F} \Phi_j \\
\frac{d}{dr} - \left( j - \frac{1}{2} + A_\phi \right) \Phi_j &= \frac{E}{\hbar v_F} \chi_j
\end{align*}
\]  

(21)

Upon solving the above set of equations for the \( r < R \), the decoupled equation is obtained as below [8]

\[ \frac{d^2\Phi_j}{dr^2} + \frac{1}{r} \frac{d\Phi_j}{dr} + \left[ k^2 - \frac{(j - 1/2)^2}{r^2} \right] \Phi_j = 0 \]  

(22)

of which the solutions can be written in terms of Bessel’s functions \( J_m(\kappa r) \) as also discussed for the scalar barrier in the previous section.

\[ \Psi_j(r, \phi) \propto \begin{cases} 
J_{j-1/2}(kr) e^{i(j - 1/2)\phi} \\
J_{j+1/2}(kr) e^{i(j + 1/2)\phi}
\end{cases} \]  

(23)

Similarly outside the dot, using \( \zeta = r^2/2 \), equations (21) reduce to the following pair of coupled linear differential equations,

\[
\begin{align*}
\left[ \frac{d}{dr} + \frac{1}{2} \left( j + \frac{1}{2} \right) + A_\phi \right] \chi_j &= \frac{1}{\sqrt{\xi}} \Phi_j \\
\left[ \frac{d}{dr} - \frac{1}{2} \left( j - \frac{1}{2} \right) + A_\phi \right] \Phi_j &= \frac{1}{\sqrt{\xi}} \chi_j
\end{align*}
\]  

(25)

where \( j = -R^2/2 \) accounts for the missing magnetic flux. Here we can recognize the solutions satisfied by confluent hypergeometric functions which are obtained as [8]

For \( j > 0 \)

\[ \Psi_j(r, \phi) \propto e^{-\sqrt{\xi} r} \begin{cases} 
\frac{k}{\sqrt{\xi}} M(\alpha, 1 + j + \frac{1}{2}; \xi e^{i(1/2)\phi}) \\
\frac{i}{\sqrt{\xi}} \frac{k}{\sqrt{\xi}} M(\alpha, 1 + j + \frac{1}{2}; \xi e^{i(1/2)\phi})
\end{cases} \]  

(26)

For \( j < 0 \)

\[ \Psi_j(r, \phi) \propto e^{-\sqrt{\xi} r} \begin{cases} 
\frac{k}{\sqrt{\xi}} M(\alpha + 1, 1 + j + \frac{1}{2}; \xi e^{-i(1/2)\phi}) \\
\frac{i}{\sqrt{\xi}} \frac{k}{\sqrt{\xi}} M(\alpha + 1, 1 + j + \frac{1}{2}; \xi e^{-i(1/2)\phi})
\end{cases} \]  

(27)

where \( M(\alpha, \beta; \xi) \) corresponds to the confluent hypergeometric functions and

\[ a = j + \frac{1}{2}, \quad a' = -k^2 \]  

(28)

(29)

We consider the charge carriers to be incident (in all directions) from inside the dot (i.e. the \( B = 0 \) region) to outside. However as shown in equation (23), the solutions inside the dot are localized Bessel’s functions. Thus, in order to carry out the analysis we decompose the Bessel’s functions in the following form of asymptotic \( (z \gg 1) \):

\[ J_m(z) \approx \frac{2}{\pi z} \left[ \cos \omega \sum_{m=0}^{\infty} \left( \frac{(-1)^m(\omega, 2m)}{(2m)!} \right) z^m - \sin \omega \left( \frac{(-1)^m(\omega, 2m + 1)}{(2m + 1)!} \right) \right] z^{-m-1/2} \]  

(30)

where

\[ \omega = \frac{1}{2} \left( 1 - \frac{1}{4\pi} \right) \]
This decomposes the wavefunction inside the dot in terms of the radially incoming and outgoing waves, so that close to the boundary we can assume the charge carriers to be incident from inside the dot towards the outside.

Next, by matching the solutions at the boundary of the dot \( r = R \), we obtain the complete normalized wavefunctions both inside and outside the dot.

3. Results and discussion

By matching the solutions at the boundary of the dot \( r = R \), we obtain the complete normalized wavefunctions both inside and outside the dot. The probability density distribution \( |\Psi(r, \phi)|^2 \) (on logarithmic base 10 scale) is plotted in figure 2. Clearly, the high probability density curves correspond to the circular regions only. This can also be understood in terms of a classical treatment in the following manner.

Since the vector potential inside the dot is zero, classically, for the electrons incident from inside the dot towards the outside, the wavevector follows a straight line to the boundary where it encounters a continuously varying vector potential and hence a refractive index. The classical trajectory bends continuously until its radial momentum vanishes (see figure 3). The classical energy-momentum relation of a massless particle moving in fields \( A \) and \( V \), with energy \( E \) and radial momentum \( p \), is

\[
\frac{p^2}{2} = \left( \frac{E - V}{\hbar v_f} \right)^2 - \left( \frac{m_l}{r} + eA_r \right)^2
\]

(31)

where the term \( \frac{m_l}{r} \) is due to the angular momentum, \( m_l = 0, \pm 1, \pm 2 \ldots \). The classical motion is restricted to the region where \( p^2 > 0 \), and \( p^2 = 0 \) defines the classical turning points [20, 21]. For our magnetic dot geometry, we obtain the classical turning points as follows. Inside the dot

\[
r = \pm \frac{m_l}{E/\hbar v_f}
\]

(32)

and outside the dot there will be two turning points obtained using the following quadratic equation:

\[
\frac{m_l}{r} + \frac{eB r^2}{2\hbar c} = \pm \frac{E}{\hbar v_f}.
\]

(33)

Expression (32) implies that for the s-wave corresponding to \( m_l = 0 \), the classical trajectories always pass through the centre of the dot. This will not be the case for higher order \( m_l > 0 \) contributions (see figure 4).

As opposed to the scalar dot in graphene where we see caustic-like features, here the probability density plot does not
show any such feature. This is also because of the underlying symmetry of the problem where the electrons are incident from inside the dot towards the outside in all directions. Unlike the scalar case the incident flux cannot be chosen in one direction from outside the barrier because the vector potential of the magnetic field extends up to infinity; also the solutions outside the dot are localized, unlike the plane wave solutions for the case of the scalar barrier. As the magnetic field is turned on the degenerate states are pulled to the closest Landau level (subband) of quantum number \( n \). Consequently, the Landau levels can be visualized by the circles, as can clearly be seen from figure 2, and the probability density at the Landau levels increases with increasing magnetic field. However, the probability density distribution inside the dot does not change to a large extent with the changing magnetic field outside the dot.

This is because the refractive index inside the dot remains the same even if we change the magnetic field outside.

This situation changes, however, if a scalar potential \( V \) is present inside the dot. The classical turning inside the dot in this case depends on the scalar potential as well.

\[
r = \pm \frac{m_i}{(E - V)/\hbar v_F}.
\]

The effective refractive index inside the dot changes due to the presence of the scalar potential \( V \), which appears in the probability density distribution plots; in addition, the sizes of the high probability density regions change with the changing scalar potential. This is clearly depicted in figure 5 as shown above.

In conclusion, we have analyzed the wavefunction probability density distribution for a magnetic dot using a full quantum mechanical calculation and also provided an explanation using a classical treatment. The solutions inside the dot are localized Bessel’s functions in nature. Using a particular form for the asymptotic we decompose these localized wavefunctions in terms of radially incoming and outgoing waves, thereby completely determining the wavefunctions inside and outside the dot. The caustic features which appear in the presence of a scalar dot in graphene are no longer present in the presence of a magnetic dot. Our results as presented may be useful for an understanding of scanning-gate microscopy on graphene quantum nanostructures. It was pointed out in earlier studies on non-relativistic 2DEG [15] that such a magnetic field profile can be realized following the work of Geim et al [22, 23]. Here the superconducting
discs with radii ranging from 0.25–1.2 μm were studied in a magnetic field in the range 50–100 Gauss. The superconducting discs were placed on top of a GaAs/AlxGa1−xAs heterostructure and the separation between the 2DEG and the superconducting disc was about 100 nm. Other methods of creating such non-uniform magnetic field profiles using hard ferromagnetic material were also discussed in a recent review [10]. These suggest that a graphene magnetic dot with well-calculated parameters can be experimentally realized. Such a magnetic dot coupled with source and drain leads via two constrictions can be used for scanning gate experiments. To illustrate this [24], has experimentally shown the imaging of resonant states of the quantum dot and the constrictions in real space. Also [25], has employed scanning tunnelling spectroscopy to study the real-space local density of states of a two-dimensional electron system in a magnetic field. We hope that our results will provide some insight and may augment the future work in this direction.

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