Electric current focusing efficiency in a graphene electric lens

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Abstract

In the present work, we study theoretically the electron wave’s focusing phenomenon in a single-layered graphene pn junction (PNJ) and obtain the electric current density distribution of graphene PNJ, which is in good agreement with the qualitative result in previous numerical calculations (Cheianov et al 2007 Science, 315, 1252). In addition, we find that, for a symmetric PNJ, 1/4 of total electric current radiated from the source electrode can be collected by the drain electrode. Furthermore, this ratio reduces to 3/16 in a symmetric graphene npn junction. Our results obtained by the present analytical method provide a general design rule for an electric lens based on negative refractory index systems.

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

The theory of negative refraction has been first analyzed by Veselago in 1968 [1]. It was suggested that a ‘perfect’ optical lens can be made based on negative refraction, which can focus light into a fine point [2]. Inspired by the analogy between ballistic electron transport in graphene and light rays in a dielectric medium, Cheianov et al proposed that an electron equivalent of negative refraction can be realized in a mono-layered graphene [3]. By fine-tuning the densities of the charge carrier on both sides of a graphene pn junction (PNJ) to be equal, the electron flow radiated from a point-like electric current source can focus exactly on the point on the other side of the PNJ due to the negative refraction of an electron wave crossing from the conduction band to the valence band. The long electron mean free path, ballistic electronic transport and high current density of graphene make graphene a good candidate for new devices based on the electric lens effect [4–8, 10, 20].

In addition to a PNJ, the electric lens of a graphene npn junction (NPNJ) is quite attractive for its potential applications in nano-electronics [3]. An electron Veselago lens of an NPNJ can be made by a graphene with two gates: one bottom gate with positive voltage is used to provide the N region in a mono-layer graphene sheet, while one top gate with negative voltage ensures the center of the graphene sheet is the P region. By carefully controlling the top gate voltage, the charge density of the P region which is between two identical N regions can be adjusted to be \( \rho_h = \rho_c \) or \( \rho_c \neq \rho_h \), and therefore affecting focusing. A graphene transistor can be achieved in an NPNJ with a rectangular-shaped top gate electrode, and a beamsplitter can be made using a prism-shaped top gate [3], which can be used to fabricate logical gates and interconnects for next-generation electronics. The principle of graphene NPNJ for a point-like electric source is similar to that of a PNJ, but has not been studied quantitatively in the literature.

To design the electric lens devices of graphene, it is necessary to analytically study the focusing phenomenon of electron flow emitted from a point-like source in a graphene...
sheet. The lack of analytical expressions of the electronic current density distribution of a PNJ and NPNJ (especially NPNJ) limits the application of graphene-based Veselago lens type devices. Moreover, the current focusing efficiency of a graphene electric lens is still an open question, which is definitely important in the design of devices. In the present work, we fulfill the task. We develop a mathematical method to get the explicit expressions for electronic current density in graphene PNJ and NPNJ. We also predict the electric current collecting efficiency of a drain electrode in the focus for symmetric PNJ and NPNJ, showing the applicability of our approach.

We start with the electronic band structure of monolayered graphene. In a graphene, carbon atoms are arranged in a honeycomb lattice, each atom connected with three nearest-neighboring atoms by covalent bonds. The $p_x$ electron of carbon atoms can form a delocalized $\pi (\pi^*)$ band, which is the valence (conduction) band of graphene, respectively. The two bands touch each other at six corners in the hexagonal Brillouin zone. For low-energy excitation near these corners, the dispersion relation of the electron is linear as $E_{c,v}(k) = \pm h v_F |k|$, which is closely similar to the energy spectrum of 2D massless Dirac fermions [11–13]. The group velocity of the electron is $V_{c,v} = \hbar \partial E/k = \pm \hbar v_F/k$ (‘$+$’ for conduction band electrons and ‘$-$’ for valence band electrons). The negative refractive index phenomenon is a consequence of different signs in the expressions of $V_{c,v}$ on two sides of the PNJ and the conservation of momentum of the wave in the direction perpendicular to the direction that the potential varies.

Ignoring the inter-valley scattering and the degree of freedom for spin, the low-energy electron in graphene can be described by a two-component spinor [14]. The effective Hamiltonian is $H = \hbar v_F \vec{\sigma} \cdot \vec{\nabla}$, with $v_F \approx c/300 \approx 10^6$ cm/s, $\vec{\sigma} = (\sigma_x, \sigma_y)$, $\sigma_x$ and $\sigma_y$ are Pauli matrices. We consider a circular source electrode with the center being located at $(-a, 0)$. The radius of the electrode should be much smaller than the size of the whole graphene sheet, but still satisfying $k_c R = 2 \pi R / k_F \gg 1$, with $k_F$ being the wavelength of the electron wave near the source electrode. The wavefunction of zero-energy electrons near the electrode can be explicitly described by a two-component spinor:

$$\psi_1(x, y) = A \left( \begin{array}{c} H_0^{(1)}(k_c r_0) e^{i\phi(x,y)} \\ i H_1^{(1)}(k_c r_0) e^{i\phi(x,y)} \end{array} \right)$$

$$\approx A \frac{2}{\pi k_c r_0} \left( \begin{array}{c} 1 \\ i e^{i\phi(x,y)} \end{array} \right) e^{ik_c r_0 - \frac{r_0^2}{2}} ,$$

(1)

which is one of a set of cylindrical function solutions of the Dirac equation in the left N region:

$$(-i\sigma_2 \partial_x - i\sigma_1 \partial_y - k_c) \psi_1(x, y) = 0 ,$$

(2)

where $A$ is a constant to be determined by a certain boundary condition and $H_0^{(1)}(z)$ is the Hankel function of the first kind. $\tan \phi = y/(x + 1)$, $r_0 \equiv \sqrt{(x + a)^2 + y^2}$ (see figure 1). Here we have used the lowest order asymptotic expansion of $H_0^{(1)}(z)$, which implies the far-field condition $k_c r_0 \gg 1$ [18] has been used [15]. It is easy to verify that only the current density of this type of wavefunction is isotropic near the edge of the source electrode, $j_{in} = e v_F \frac{1}{\pi} \cos \phi$, while all other cylindrical function solutions give $j_{in} \sim (\sin \theta, \sin \phi, n \geq 2$. Given the input current $I_0$, the continuity of electric current at the boundary of the source electrode implies $I_0 = 2\pi R_j|_{in}$, which determines constant $A = \sqrt{k_c R_0 / (8\pi v_F)}$. We consider the PNJ and NPNJ in a large graphene sheet, with absorbing boundary condition. Thus a part of the electronic current does not transport across the junction. Instead, it hits the edges of graphene sheet and is then absorbed by the boundaries.

The penetration problem of an incident plane wave of an electron at interfaces of the PNJ and NPNJ in graphene has already been studied in the literature [3, 16]. To use these results in the present case of a cylindrical incident wave, the key point is to find a suitable expansion of the cylindrical wave in a set of plane wave basis, i.e. describe the cylindrical wave as the superposition of a series of plane waves. Then we will use the results for refraction (for PNJ) and transmission (for NPNJ) of each plane wave components of an incident wave, then add them together to obtain the whole refractive (transmitted) electron wave.

The expansion of an incident cylindrical electron wave as given in equation (1) can be rewritten as [17]

$$\psi_1(r_1) = \frac{A}{\pi} \int_{-\infty}^{\varphi_0} e^{i k_c x \cos \theta_c} \left( \begin{array}{c} 1 \\ e^{i\theta_c} \end{array} \right)$$

$$\times e^{ik_c(x \cos \theta_c + y \sin \theta_c)} d\theta_c .$$

(3)

In general, the contour of the integral is shown in figure 2(a). Here, $\bar{k}_c \equiv (k_c \cos \theta_c, k_c \sin \theta_c)$ is the wavevector of the incident electron wave component with incident angle $\theta_c$.

At first, we study the refraction of a PNJ, which is shown in the sketch in figure 1. We know a plane wave with the angle of incidence $\theta_c$ has a form [14]

$$\psi_{plane-in} = \left( \begin{array}{c} 1 \\ e^{i\theta_c} \end{array} \right) e^{ik_c(x \cos \theta_c + y \sin \theta_c)} ,$$

Figure 1. The schematic diagram for electric lens in symmetric graphene PNJ. The electric current source is located at $(-a, 0)$. The electron flow radiated from the current source focuses at the P region.
which reflects and refracts at the interface of the PNJ, with the reflected wave and refractive wave being
\[ \psi_{\text{plane-ref}}(x, y) = \frac{1}{\sqrt{2}} \left( \frac{1}{e^{i(\pi - \theta_i)}} \right) e^{i k_c (-x \cos \theta_i + y \sin \theta_i)}, \]
and
\[ \psi_{\text{plane-ref}}(x, y) = \frac{1}{\sqrt{2}} \left( \frac{1}{e^{i \theta_i}} \right) e^{-i k_c (x \cos \theta_i + y \sin \theta_i)}, \]
respectively. Here, three wavefunctions \( \psi_{\text{plane-ref}}(x, y) \), \( \psi_{\text{plane-ref}}(x, y) \) and \( \psi_{\text{plane-ref}}(x, y) \) are the plane wave solutions of the Dirac equations
\[ \begin{cases} 
( -i \sigma_x \partial_x - i \sigma_y \partial_y + k_c ) \psi(x, y) = 0, & x < 0 \\
( -i \sigma_x \partial_x - i \sigma_y \partial_y - k_c ) \psi(x, y) = 0, & x > 0.
\end{cases} \] (4)
The factor \( e^{i \pi} \) in the reflected wavefunction \( \psi_{\text{plane-ref}}(x, y) \) is related to the Berry phase [14].

By the continuity of the wavefunction in the N region and P region
\[ \psi_{\text{plane-in}}(0, y) + r \psi_{\text{plane-ref}}(0, y) = r \psi_{\text{plane-ref}}(0, y), \]
the coefficient of refraction can be obtained easily as \( r = 2 \cos \theta_i / (e^{i \theta_i} + e^{-i k_c}) \), and the coefficient of reflection is therefore \( r = 1 - t \).

The refractive wavefunction of a cylindrical wave is therefore
\[ \psi_{\text{refr}}(x, y) = \frac{A}{\pi} \int_{-\infty}^{\infty} e^{i k_c \cos \theta_i} \frac{2 \cos \theta_c}{\sin \theta_c} \left( e^{i k_c r_1 \cos \theta_i - (\pi - \alpha)} \right) \frac{1}{e^{i \theta_i}} e^{-i k_c (x \cos \theta_i + y \sin \theta_i)} \, dx, \quad x > 0. \] (5)

Momentum conservation in the y direction requires \( k_c \sin \theta_c = -k_y \sin \theta_i \), which implies the relation between the angle of refraction \( \theta_l \) and the angle of incidence \( \theta_i \), which is similar to the Snell’s law in optical refraction [3]:
\[ \frac{\sin \theta_c}{\sin \theta_i} = \frac{-k_y}{k_c} \equiv n. \] (6)

For simplification, we study the refraction for a symmetric PNJ at first, then study the asymmetric PNJ with \( n \neq 1 \). For convenience, we shift the integral contour as shown in figure 2(b) for a symmetric case, i.e. \( k_r = k_c, n = -1 \), and \( \theta_i = -\theta_c \), the refractive wave at the P region has a simple form:
\[ \psi_{\text{refr}} = \frac{A}{\pi} \int_{-\infty}^{\infty} d\cos \theta_c \left( e^{i k_c} \right) e^{i k_r \cos (\theta_i - (\pi - \alpha))} \]
\[ \approx \frac{A}{\pi} \left[ 2 \pi k_c r_1 \right] e^{-i k_r \cos (\pi - \alpha)} \] (7)
\[ \times \left( e^{i k_r \cos (\pi - \alpha)} \right) \cos \alpha, \]
\[ \alpha \in \left[ \frac{\pi}{2}, \frac{3\pi}{2} \right]. \] (8)

Here, \( \tan \alpha = \gamma / (x - a) \) and \( r_1 = \sqrt{(x - a)^2 + y^2} \). We have used the steepest descent method with the inclusion of only one leading term [17], which implies the approximate refractive wavefunction in equation (8) is valid for \( k_r r_1 \gg 1 \). Since \( \lambda_F \), the wavelength of the electron in graphene is at most several nanometers and the far-field condition \( k_r r_1 \gg 1 \) is reasonable, thus the results obtained by the present approximation are also reasonable.

The current density \( \vec{j} = e v_F \psi_{\text{refr}}^\dagger \vec{\sigma} \psi_{\text{refr}} \) is therefore
\[ \vec{j}_z(r_1, \alpha) (k, R) \]
\[ \approx \left\{ \begin{array}{ll}
\frac{I_0}{2 \pi r_1} \cos^2 \alpha & \cos \alpha, (\sin \alpha), \\
\alpha \in [-\pi/2, \pi/2], \\
\frac{I_0}{2 \pi r_1} \cos^2 \alpha & \cos \alpha, (\sin \alpha), \\
\alpha \in [\pi/2, 3\pi/2].
\end{array} \right. \] (9)

The intensity of current density around, but not too close to, the focus \((a, 0)\) has an expression \( j_1 \propto \cos^2 \alpha / r_1 = \).
Figure 3. Intensity distribution of current density in the P region of a graphene PNJ ($x \geq 0$). $x$, $y$ coordinates are in units of $a$. (a) $n = -1$, focus is located at $(a, 0)$, (b) $n = -1.2$, refracted wave forms a caustic, with the cusp located at $(1.2a, 0)$.

$(x - a)^2 / [(x - a)^2 + y^2]^{3/2}$, as shown in figure 3(a), which is in agreement with the corresponding result in [3].

If a detecting circular electrode with radius $R$ is placed at $(a, 0)$, the maximal electric current that can be collected by it can be obtained as

$$I = R \int_{\pi/2}^{3\pi/2} \mathbf{j}(R, \alpha) \cdot (\cos \alpha, \sin \alpha) = \frac{I_0}{4}. \quad (10)$$

Thus only 1/4 of the total current from the source electrode can be collected by the detecting drain electrode. A graphene electronic lens device should be sophisticatedly designed for high efficiency.

In general, an asymmetric PNJ leads to a refraction index $n \neq -1$; the refractive wavefunction does not have a simple form. The integral in equation (5) can still be calculated by the steepest descent method. The results for $n = -1.2$ are shown in figure 3(b). As discussed in [3, 18], electron flow transporting across an asymmetric PNJ forms caustics, with the cusp located at $(|n|a, 0)$. Our results shown in figure 3(b) are in good agreement with those in [3].

In the original prediction of an optical Veselago lens, the electromagnetic wave from a point-like source focuses on a point after transmitting across negative refraction material, which is in close analogy with the focusing of electron flow at the second N region in the graphene NPNJ, as shown in figure 4.

Using a similar method for the refractive wave of graphene PNJ, we firstly find each plane electron wave component of the transmission wave, then ‘add’ all the components together (in fact, by an integral). The plane wave’s transmission across the P region between two N regions can be solved by the standard method for an electron wave transmitting across a square energy barrier [11, 16].

We separate the 2D space in graphene NPNJ into three regions $x \leq 0$, $0 \leq x \leq d$ and $x > d$, labeled by I, II and III, respectively. The Dirac equations for the three regions of an NPNJ are

$$(-i\sigma_x \partial_x - i\sigma_y \partial_y + k_c) \psi(x, y) = 0,$$

$$x \leq 0 \quad \text{or} \quad x \geq d$$

$$(-i\sigma_x \partial_x - i\sigma_y \partial_y - k_c) \psi(x, y) = 0, \quad 0 \leq d. \quad (11)$$

The plane wavefunction at each region is the solution of equation (11), which can be written as

$$\psi_1(x, y) = \frac{1}{\sqrt{2}} \left( \begin{array}{c} 1 \\ e^{i\theta_x} \end{array} \right) e^{ik_c \cos \theta_x x + ik_c \sin \theta_y y} + \frac{r}{\sqrt{2}} \left( \begin{array}{c} 1 \\ -e^{-i\theta_x} \end{array} \right) e^{-ik_c \cos \theta_x x + ik_c \sin \theta_y y}, \quad x < 0,$$
ψ_{III}(x, y) = \frac{t}{\sqrt{2}} \left( \frac{1}{e^{i\theta_c}} e^{-ik_c x - ik_c y} \right) e^{i(k_c x - y \theta_c)} \left( \frac{1}{e^{i\theta_c}} e^{ik_c x + ik_c y} \right) e^{-i(k_c x + y \theta_c)}.

Thus, the transmission wave at the second N region can be written as

$$\psi_{\text{transmission}}(x, y) \approx \begin{cases} \sqrt{\frac{2}{\pi k_c r_2}} \cos^2 \beta \left( \frac{1}{e^{i\theta_c}} e^{ik_c x - \pi/4} \right), & \beta \in \left[ -\frac{\pi}{2}, \frac{\pi}{2} \right] \\ \sqrt{\frac{2}{\pi k_c r_2}} \cos^2 \beta \left( \frac{1}{e^{-i\theta_c}} e^{-ik_c x - \pi/4} \right), & \beta \in \left( \frac{\pi}{2}, \frac{3\pi}{2} \right] \end{cases} \tag{14}$$

Here, $a_1 = 2d - a$. At the second N region (region III), the electric current density around the point $(a_1, 0)$ is

$$j_2 = |\bar{j}(x, y)| = \frac{I_0}{2\pi} \frac{(x - a_1)^4}{(x - a_1)^2 + y^2} \sqrt{\frac{2}{\pi k_c r_2}}.$$

![Figure 5. Intensity distribution of current density in second N region (x ≥ d) of a graphene NPNJ. The x and y coordinates are measured from the focus located at (2d – a, 0), in units of a.](image-url)
devices, such as predicting the theoretical upper bound of efficiency for realistic devices.

In summary, we have theoretically reproduced the electric lens phenomena in graphene PNJ and NPNJ, and have obtained the analytical expressions for the current density distribution in a PNJ and NPNJ. The key idea is to expand the incident cylindrical wave in a series of plane wave basis, then find the refractive wave or transmitted wave for each incident plane wave component, adding them together and getting the total refractive wave (in a PNJ) and transmitted wave (in an NPNJ), as shown in equations (9) and (15), figures 3 and 5. The analytical results are in good agreement with available numerical results in [3]. We firstly obtained the maximal possible current which can be collected by the drain electrode in a symmetric PNJ and NPNJ, which are $1/4$ and $3/16$, respectively. These data are important in designing devices, such as logical gates and interconnects based on a graphene Veselago lens.

Recent progress on the flat-lens focusing of electrons on the surface of a topological insulator suggested a highly efficient electric lens effect based on a topological insulator [23]. In this electric lens, only conduction band electrons are used, which avoids high interface resistance in graphene PNJ. We are now working on the possibility of applying our theory to this interesting issue.

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