disorder-induced enhancement of transport through graphene p-n junctions

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We investigate the electron transport through a graphene p-n junction under a perpendicular magnetic field. By using Landauer-Buttiker formalism combining with the non-equilibrium Green function method, the conductance is studied for the clean and disordered samples. For the clean p-n junction, the conductance is quite small. In the presence of disorders, it is strongly enhanced and exhibits plateau structure at suitable range of disorders. Our numerical results show that the lowest plateau can survive for a very broad range of disorder strength, but the existence of high plateaus depends on system parameters and sometimes cannot be formed at all. When the disorder is slightly outside of this disorder range, some conductance plateaus can still emerge with its value lower than the ideal value. These results are in excellent agreement with the recent experiments.

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Due to the recent success in fabrication of graphene, a single-layer hexagonal lattice of carbon atoms, great attention has been attracted in the research of graphene. The unique band structure of graphene with a linear dispersion relation \(E = \pm h c |k|\) near the Dirac-points leads to many peculiar properties. For instance, the quasi-particles obey the Dirac-like equation and have the relativistic-like behaviors with zero rest mass. Its Hall plateaus assume the half-integer values for the p-p junction. By varying the gate voltage, the carrier of graphene can be tuned from electron-like to hole-like and vice versa. To examine the interplay between the electron-like and hole-like quasi-particles, a graphene p-n junction would be a good candidate. Many exciting phenomena reflecting the massless Dirac character of carriers, such as relativistic Klein tunneling and Velselago lensing, were predicted for the graphene p-n junction.

Very recently, the graphene junction has been realized experimentally. As expected, it was found that in quantum Hall regime the two-terminal conductance exhibits quantized plateaus with half-integer values for the p-p or n-n junctions. For the disordered p-n junction, new plateaus emerge at \(e^2/h\) and \((3/2)e^2/h\). At the same time, a theoretical analysis qualitatively explained the appearance of these plateaus that is due to the mixture of the electron and hole Hall edge modes in the p-n boundary. After that, subsequent works have also investigated the graphene p-n junction. However, these theories can not account for the experimentally observed plateau that appeared at about 1.4\(e^2/h\) which is lower than the expected value \((3/2)e^2/h\). In addition, the reason that the expected plateaus at 3\(e^2/h\) or higher values have not been observed remained mysterious. In view of this situation, it is clear that a quantitatively analysis for the graphene p-n junction is needed.

In this paper, we theoretically study the electron transport through the p-n junction of disordered graphene under a perpendicular magnetic field \(B\). By using the tight-binding model and the Landauer-Buttiker formalism combining with the non-equilibrium Green function method, the conductance is calculated in both clean and disordered samples. Numerical results show that the conductance is very weak in the clean p-n region at large \(B\). With increasing of the disorder, the conductance is strongly enhanced and new plateaus emerge at \(e^2/h, (3/2)e^2/h, \ldots\) etc. The range of the disorder strength \(W\) needed for the existence of the lowest plateau \(e^2/h\) is very broad, so this plateau can easily be observed. But for the plateaus corresponds to higher quantization values, the range of \(W\) can be very narrow. Sometimes these higher order plateaus can not be formed. Our results seem to suggest that the higher the plateau value, the more difficult it is to observe experimentally. When the disorder is slightly off this disorder range, the conductance plateaus can still emerge, but its value is lower than the expected one. These results are in excellent agreement with experimental data.

In the tight-binding representation, the Hamiltonian of the graphene p-n junction (see Fig.1a) is given by:

\[
H = \sum_i \epsilon_i a_i^\dagger a_i - \sum_{\langle ij\rangle} t e^{i\phi_{ij}} a_i^\dagger a_j
\]

where \(a_i^\dagger\) and \(a_i\) are the creation and annihilation operators at the discrete site \(i\), and \(\epsilon_i\) is the on-site energy. In the left and right leads, \(\epsilon_i = E_L\) or \(E_R\), which can be controlled by the gate voltages. The disorder exists only in the center region. The potential drop from the right to the left leads is assumed to be linear, i.e., \(\epsilon_i = k(E_R - E_L)/(2M + 1) + E_L + w_i\), where \(M\) is the length of the center region and \(k = 0, 1, 2, \ldots 2M + 1\) (see Fig.1a). The on-site disorder energy \(w_i\) is uniform distributed in the range \([-W/2, W/2]\) with the disorder strength \(W\). The size of the center region is described by the width \(N\) and length \(M\), and it has \(2N(2M + 1)\) carbon atoms. In Fig.1a, it shows a system with \(N = 2\) and
$M = 4$. Here we only consider the zigzag edge graphene, but all results are similar for the armchair edge graphene. The second term in Hamiltonian (1) describes the nearest neighbor hopping. Due to the existence of the perpendicular magnetic field $B$, a phase $\phi_{ij}$ is added in the hopping element, and $\phi_{ij} = \int_{i}^{j} A \cdot d\ell/\phi_0$ with the vector potential $\vec{A} = -(B_y, 0, 0)$ and $\phi_0 = h/e$.

The current flowing through the graphene p-n junction is calculated from the Landauer-Büttiker formula \[ I = (2e/h) \int dc \, T_{LR}(\epsilon) f_L(\epsilon - f_R(\epsilon)), \] where $f_\alpha(\epsilon) = 1/\exp[(\epsilon - eV_\alpha)/k_BT + 1]$ ($\alpha = L, R$) is the Fermi distribution function in the left and right graphene lead. Here $T_{LR}(\epsilon) = Tr[\Gamma_L G^R \Gamma_R G^L]$ is the transmission coefficient, where the linewidth functions $\Gamma_\alpha(\epsilon) = i[\Sigma^\prime_\alpha(\epsilon) - \Sigma_\alpha^{\prime\prime}(\epsilon)]$, the Green functions $G^\alpha(\epsilon) = [G^\alpha(\epsilon)]^\dagger = 1/[\epsilon - \vec{H}_{cen} - \Sigma^\prime_\alpha - \Sigma_\alpha^{\prime\prime}]$, $\vec{H}_{cen}$ is the Hamiltonian in the center region, and $\Sigma^\prime_\alpha$ is the retarded self-energy due to the coupling to the lead-\(\alpha\) that can be calculated numerically. After obtaining the current $I$, the linear conductance is given by $G = \lim_{V \to 0} dI/dV$.

In the following numerical calculations, we use the hopping energy $t \approx 2.75eV$ as the energy unit. Since the hopping energy $t$ corresponds to $10^4K$, we can safely set the temperature to zero in our calculation. The width $N$ is chosen as $N = 50$ in all calculations. Since the nearest-neighbor carbon-carbon distance $a = 0.142nm$, the width is $3aN = 21.6nm$ for $N = 50$. The magnetic field is expressed in terms of $\phi$ with $\phi = (3\sqrt{3}/4)a^2B/\phi_0$ and $(3\sqrt{3}/2)a^2B$ is the magnetic flux in the honeycomb lattice. In the presence of the disorder, the conductance is averaged over up to 2000 random configurations except for Fig.2b where only 400 random configurations were used for each data. In the experiment, the typical concentration of electrons or holes is around $10^{13}cm^2$ that corresponds to the on-site energies $E_L, E_R \leq 0.1t$. So we will mainly focus on the region of $E_L$ and $E_R$ within 0.3$t$.

In this range of $E_L$ or $E_R$, the dispersion relation is linear and exhibits Dirac behaviors.

We first study the clean graphene junction. Fig.1b and c show the conductance $G$ versus the Fermi level of right lead $E_R$ setting the magnetic field $B = 0$. In the n-n region with $E_L, E_R < 0$, $G$ is approximatively quantized and exhibits a series of equidistant plateaus at the half-integers (in the unit of $4e^2/h$) due to the transverse sub-bands of the lead with finite width. Because of the linear dispersion relation the transverse sub-bands $E_n$ of the confined graphene are in equidistant instead of $E_n \sim n^2$ of the usual two-dimensional electron gas. While for $E_R < E_L$, due to the fixed sub-band numbers in the left region, no more higher plateaus appear. On the other hand, in the p-n region with $E_L < 0$ and $E_R > 0$, there is no plateaus. The conductance $G$ in the p-n region ($E_R > 0$) is always less than the corresponding plateau value in the n-n region ($E_R < 0$). Due to the occurrence of the Klein tunneling processes, the conductance is quite large, e.g., $G > e^2/h$ for almost all positive $E_R$ at $M = 5$. With the increase of $M$, the Klein tunneling processes are slightly weakened and so is the conductance.

Next, we examine the effect of the magnetic field $B$ in the clean sample. With the increase of $B$, the equidistant sub-bands gradually evolve into the Landau levels which scales as $E_n \approx \sqrt{n}$ for the Dirac particle. The conductance plateaus in the n-n region evolve into the Hall plateau, and the conductance $G$ in the p-n region is strongly suppressed at small $E_R$. Fig.1d,e and Fig.2a show $G$ at a high magnetic field with the magnetic flux (or phase) $\phi = 0.007$. We see perfect Hall plateau in the n-n junction with equidistant in the scale of $E_R^2$ (see Fig.2a). The plateau values are given by $\min(|\nu_L|, |\nu_R|)2e^2/h$ where $\nu_\alpha$ is the filling factors in the lead-\(\alpha\). In particular the Hall plateaus, i.e. the curve of $G-E_R$ in Fig.1d and 1e at $E_R < 0$, do not depend on $M$. However, in the p-n region ($E_R > 0$ and $E_L < 0$), no plateaus exist. The conductance $G$ is small and strongly depends on the junction length $M$. For the small filling factors $\nu_L$ and $\nu_R$ or the large junction length $M$, $G$ is almost zero. This is because for the clean p-n junction, the Hall edge states for electrons and holes are well separated in the space and do not form the mixture of the states leading to the very small conductance.

In the following, we shall focus on how the conductance $G$ is affected by the disorders. Fig.2 plots $G$ versus the energy $E_L$ and $E_R$ with the disorder strength $W = 0$ and $W = 2$. In the presence of disorders, the conductance $G$ in the p-n region (or n-p region) is strongly enhanced due to the mixture of the electron and hole Hall edge states, while $G$ in the n-n and p-p regions are slightly weakened. At fixed filling factors $\nu_L$ and $\nu_R$, $G$ is approximatively a constant. As $\nu_L$ or $\nu_R$ varies, a jump occurs in $G$ with the borders between $\nu_L$ and $\nu_R$ regions clearly seen in Fig.2b.

Now we investigate the effect of disorders on the conductance in more detail. Fig.3 depicts the conductance vs $E_R$ at fixed $E_L = -0.1$ ($\nu_L = -2$) and $-0.2$ ($\nu_L = -6$). When $W = 0$, $G$ is small in the p-n region and $G$ exhibits the Hall plateaus in the n-n region. With the increase of $W$ from 0, the conductance $G$ in the p-n region is strongly enhanced even for very small $W$. For example, for $W = 0.02$ or $W = 0.05$, $G$ is greater than $0.2e^2/h$, which is much larger than that ($G < 0.001e^2/h$) at $W = 0$ (see Fig.3a,c). When $W = 0.1$, the lowest conductance plateau with $\nu_L = -2$ and $\nu_R = 2$ is well established with its plateau value at $e^2/h$. In particular, this plateau remains for a broad range of disorder strength $W$ (from 0.1 to 3). For the higher filling factors, the conductance is also enhanced by the disorder, but it requires much large disorder to reach its ideal plateau value at $|\nu_L||\nu_R|/(|\nu_L| + |\nu_R|)e^2/h$. For example, for $\nu_L = -2$ and $\nu_R = 6$ or $\nu_L = -6$ and $\nu_R = 2$, the conductance reaches the plateau of $(3/2)e^2/h$ when $W = 2$ (see Fig.3b,d). In the n-n region, the Hall plateau is not affected by the small disorders and kept their values at $\min(|\nu_L|, |\nu_R|)e^2/h$. If the disorder strength $W$ is increased further, the conductance $G$ starts to drop in both n-n and p-n regions. For very large $W$ (e.g. $W = 6$ or
larger), the system enters the insulating regime and $G$ is very small for all $E_L$ and $E_R$. Here we wish to emphasize two points: (i). We have seen that the new plateau survives only within certain range of $W = [W_{\text{min}}, W_{\text{max}}]$. When the disorder is slightly below $W_{\text{min}}$ or above $W_{\text{max}}$, the conductance $G$ still exhibits a plateau but its value is less than the value of ideal plateau. For example, the plateau of $\nu_L = -2$ and $\nu_R = 6$ is less than $(3/2)e^2/h$ when $W = 1$ and $W = 3$ (see Fig.3c and 3d). (ii). For some high filling factor region (e.g. $\nu_L = -6$ and $\nu_R = 6$), the conductance plateau does not emerge at all for any $W$. Because it is much more difficult to completely mix all states for high filling factor case, so the system goes to the insulating regime before the occurrence of the complete state mixture. These numerical results are in excellent agreement with the experiment.

We now focus on the conductance vs disorder strength for energies $E_L$ and $E_R$ shown in Fig.2a (solid dots). In the p-n region, the Hall edge states are very robust against disorders so the conductance remains quantized at small $W$ (see Fig.4b). At large disorders, the edge states are destroyed and the Hall conductance monotonically decreases with increasing of $W$. In the p-n region (Fig.4a,c and d), the enhancement of conductance due to fluctuations when the edge states are partially destroyed. For the lowest filling factors with $\nu_L = -2$ ($E_L = -0.1$) and $\nu_R = 2$ ($E_R = 0.1$), $G$ reached its ideal plateau value $e^2/h$ at $W = 0.09$ and stayed there until $W = 3$ (see Fig.4a). We emphasize that this range of disorder $W$ (from 0.09 to 3) is very broad, extends in almost two orders of magnitude! So the lowest plateau can easily be observed experimentally. For $\nu_L = -2$ and $\nu_R = 6$ ($E_R = 0.2$) (or $\nu_R = 10$ with $E_R = 0.25$), the left side of the sample has an electron Hall edge state and the right side has three (or five) holes Hall edge states. As a result of the mixture of the left-side electron state and one of right-side hole states, the conductance $G$ develops a step around $e^2/h$. Upon further increasing $W$, the complete mixture of the left-side electron state and all right-side hole states occurs at $W = 1.6$ (or 1.7) and the conductance $G$ reaches the ideal plateau value $(3/2)e^2/h$ (or $(5/3)e^2/h$). Note that this ideal plateau exists only within the disorder window $1.7 < W < 2.6$ (or $1.6 < W < 2.4$) that is much narrower than that of the lowest plateau. Our results also show that for the case of higher filling factors (e.g. $\nu_L = -6$ and $\nu_R = 6$), the ideal plateau $3e^2/h$ can not be reached for any disorders. When the center region becomes longer or shorter, the conductance $G$ shows similar results (see Fig.4c,d). For a short center region (e.g. $M = 10$), the conductance reaches the ideal lowest plateau at a larger $W$ with a smaller plateau width. The high conductance plateau at $\nu_L = -6$ and $\nu_R = 6$ also appears. On the other hand, for a longer center region (e.g. $M = 40$), $G$ reaches the ideal lowest plateau at a smaller $W$ with a wider plateau. Except for the lowest plateau, all other plateaus (including $(3/2)e^2/h$ and $(5/3)e^2/h$) do not appear for $M = 40$.

Finally, we study the conductance fluctuation $rms(G) \equiv \sqrt{(G - \langle G \rangle)^2}$, where $\langle ... \rangle$ is the average over the disorder configurations with the same disorder strength $W$. Fig.5 shows $rms(G)$ versus $W$ with the same set of parameters as in Fig.4a and 4b. In the n-n region (see Fig.5b), there is no fluctuation of the Hall edge states at small $W$. When disorder increases, the conductance fluctuates when the edge states are partially destroyed. At large disorders, $rms(G)$ eventually goes to zero and enters the insulating regime. On the other hand, in the p-n region (see Fig.5a), the fluctuation $rms(G)$ is small for both small and large $W$. But $rms(G)$ is large for intermediate $W$ and usually exhibits a double-peak structure. In particular, $rms(G)$ does not have the plateau although the conductance has a very long plateau especially at $\nu_L = -2$ and $\nu_R = 2$.

In summary, the electron transport through a graphene p-n junction under the perpendicular magnetic field is numerically and quantitatively studied. We find the conductance is quite small for the clean p-n junction. But the disorder can drastically enhance the conductance leading to the conductance plateaus. The lowest conductance plateaus can sustain for a very broad range of disorder strength (about two orders of magnitude), but the higher plateaus are difficult to form. When the disorder is slightly outside of this disorder range, some conductance plateaus in $G$ vs $E_R$ curve can also emerge with plateau value smaller than the ideal value.

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FIG. 1: (Color online) (a). The schematic diagram for a zigzag edge graphene p-n junction. (b), (c), (d), and (e): the conductance $G$ vs $E_R$ for different center lengths $M$ at $W = 0$. The parameters $E_L = -0.1$ for (b) and (d) and $E_L = -0.2$ for (c) and (e), and $\phi = 0$ for (b) and (c) and $\phi = 0.007$ for (d) and (e).

FIG. 2: (Color online) The conductance $G$ (in the unit of $2e^2/h$) vs $E_L$ and $E_R$ with $M = 20$, $\phi = 0.007$. (a): $W = 0$ and (b): $W = 2$.

FIG. 3: The conductance $G$ vs $E_R$ for the different disorder strengths $W$, with the parameters $M = 20$, $\phi = 0.007$. (a) and (b): $E_L = -0.1$. (c) and (d): $E_L = -0.2$. 
FIG. 4: The conductance $G$ vs disorder strength for $E_L$ and $E_R$ fixed at different points shown in Fig. 2a with $\phi = 0.007$. The system size, $M = 20$ for (a) and (b), $M = 10$ for (c), and $M = 40$ for (d). $E_L$ and $E_R$ in (a) and (c) are same as in (d).

FIG. 5: $rms(G)$ vs $E_R$. The parameters in (a) and (b) are the same as in Fig. 4a and 4b, respectively.
