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Uncovering the dominant scattering mechanism in graphene system

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ABSTRACT

We re-investigate the impact of possible scattering mechanism on quantum transport properties in graphene. For Coulomb scatters, conductivity-carrier-dependence $\sigma(n)$ away from the Dirac point can vary from sub-linear to linear behavior with increasing the impurity concentration, which is consistent with the existed experimental observations. For comparison, we also confirm that the resonant impurities or ripples cannot produce a linear behavior conductivity-carrier-dependence. Therefore, our results indicate that main scattering mechanism in samples with linear behavior of $\sigma \propto n$ comes from the Coulomb charged impurities. While the sub-linear behavior in other samples may result from the above three scattering mechanisms.

1. Introduction

Graphene has been attracting a lot of attentions for its remarkable properties and for its potential applications in nanoelectronics [1]. To fabricate electronic devices with high mobility requires a comprehensive understanding of the effect of disorder on the transport properties of graphene. Thus the question what kind of disorder mainly limits the mobility of charge carriers in graphene has invoked an intense debate after the first transport measurement [2,3]. There are two key findings in initial experiment [4]: 1) the conductivity σ increases linearly with the carrier density n away from the Dirac point; 2) a minimal conductivity $\sigma_{\min}$ seems a quasi-universal value $\sim 4e^2/h$. Nevertheless, after that, many groups found a sub-linear relationship between σ and n in their samples and a sample (mobility) dependent value of minimal conductivity [5–12]. The above discrepancy existed in the experiments also needs a plausible understanding.

On the theoretical side, how to understand the transport properties in graphene is still an open question and no consensus has been reached so far. For example, some authors [13] developed a modified semiclassical Boltzmann theory to study the effects of Coulomb scatters on transport properties. Nevertheless, quantum interference effects due to potential fluctuation are missing so that Boltzmann theory cannot capture the important graphene's transport behaviors near the Dirac point [3]. Adam et al. [14] showed both the Boltzmann theory and the Landauer approaches lead to $\sigma \propto n^{3/2}$ away from the Dirac point for the case of the correlated Gaussian potential. This, however, disagrees with all experimental observations reported so far [4–9] and previous Landauer-type numerical calculations [15–18]. K. Nomura et al. [19] employed a calculation in momentum-space to show that Coulomb scatters are able to account for the linear dependence in graphene. But the predicted universal behavior of conductivity with non-sensitive to the strength of disorder is also at odds with many experiments [5,6,8,9]. And the naive cut-off in momentum-space is also deserved debate. Moreover, some alternative explanations to experiment based on resonant impurities and ripples are also proposed. T. Stauber et al. [20] proposed that resonant impurities can account for the sub-linear behavior of the conductivity versus charge density: $\sigma_{xx} \propto n \ln^2 |\frac{E_F}{D}|$. M.I. Katsnelson et al. [21] pointed out that the certain types of microscopic corrugations in graphene can create a long-ranged scattering mechanisms similar to Coulomb scatters and result in linear dependence of conductivity on charge carriers. But this conclusion is also under debate [3]. To sum up, although the main origin of scattering mechanism has spurred a vast amount of theoretical work, to date, the answer remains elusive and no theory has been able to render a full picture of this puzzle [22–27].

In this Letter, we perform a large-scale calculation in real-space based on the Kubo formula to study the effect of extrinsic and intrinsic disorder on the transport properties of graphene. The particular advantage of our method is unnecessary for making any assumption about the underlying dynamical regime or introducing any energy cut-off. In order to compare with experiments, we restrict ourselves in the realistic range of impurities concentration $10^{11}\ \text{cm}^{-2} < n_{imp} < 10^{13}\ \text{cm}^{-2}$ and the available carrier density $n < 10 \times 10^{12}\ \text{cm}^{-2}$ reported in experiments. Our results confirm that, taking into account Coulomb scatters with

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high impurity concentration can produce the linear carrier-density-dependent conductivity in experiments. We also find that there is a quantum interference regime near the Dirac point where the conductivity will be enhanced by disorder owing to the quantum interference effect. This finding gives a natural interpretation to the existed experiments such as [4–8]. Furthermore, we compare the Coulomb scatters with the resonant impurities and ripples. It is found that the resonant impurities or ripples can only result in a sub-linear dependence of conductivity on carrier density and relative low value of minimal conductivity $< 4e^2/h$. We believe that our results have clarified the different role of scattering mechanism in transport properties in graphene.

The remainder of this Letter is organized as follows. In Section 2 we introduce the model and method used for calculation. In Section 3, we show our calculated conductivity for Coulomb impurities randomly distributed on graphene sheet. We focus on the relationship between conductivity and carrier density and minimal conductivity behavior. The related experimental observations and derivation from previous theoretical predictions are also discussed. In Sections 4 and 5, we draw some comparisons with the cases with resonant impurities and ripples, respectively. Discussion and conclusions are given in Section 6.

2. Model and method

Low energy excitations of graphene come from the π-electrons that can be modeled by a tight-binding Hamiltonian on a honeycomb lattice,

$$H = \sum_{\langle ij\rangle} t_{ij}|i\rangle\langle j| + \text{h.c.} + \sum_i \epsilon_i |i\rangle\langle i| \tag{1}$$

where $|i\rangle$ denotes the π-electron state on site i. $t_{ij} = t_0 = -2.7$ eV is the hopping energy between two nearest-neighbor sites. The effects of ripples will change the distance between two nearest-neighbor sites therefore changes the hopping energy t_{ij}. $\epsilon_i = V(\mathbf{r}_i)$ is the on-site energy mimic the potential induced by Coulomb impurities.

As noted before, here we focus on the numerical calculation of the dc conductivity of disordered graphene system. Within linear response the Kubo formula for the conductivity is written as:

$$\begin{aligned}\sigma_{xx} &= \frac{2\hbar}{\pi L^2}\lim_{\omega\mapsto 0}\int_{-\infty}^{\infty} dE\,\frac{f(E)-f(E+\hbar\omega)}{\hbar\omega} \\ &\quad\times Tr\big[\hat{j}_x Im\,\hat{G}^R(E)\hat{j}_x Im\,\hat{G}^R(E+\hbar\omega)\big] \\ &= \frac{2\pi\hbar}{L^2}\lim_{\omega\mapsto 0}\int_{-\infty}^{\infty}\frac{f(E)-f(E+\hbar\omega)}{\hbar\omega}J(E,E+\hbar\omega)\,dE\end{aligned} \tag{2}$$

where e is electron charge and $\hbar$ is the Planck constant and L^2 stands for area of graphene. $f(E)$ is Fermi–Dirac distribution function and we only focus on zero temperature limit here. $\hat{G}^R(E) = \frac{1}{E-H+i0^+}$ is the retarded Green's function of the disordered system. $\hat{j}_x = -i\sum_{j,\delta} t_{ij}(\mathbf{e_x}\cdot\delta|\mathbf{j}\rangle\langle\mathbf{j}+\delta| - \mathbf{e_x}\cdot\delta|\mathbf{j}+\delta\rangle\langle\mathbf{j}|)$ is the x component of the current operator (defined through the Heisenberg equation-of-motion for the position coordinate). $J(E,E+\hbar\omega) = Tr[\hat{j}_x\delta(E-\hat{H})\hat{j}_x\delta(E+\hbar\omega-\hat{H})]$ is current–current correlation function. Eq. (2) involves a summation over matrix elements between all one-particle eigenstates of Eq. (1), which can hardly be calculated for a reasonably large system. To overcome these complications we employ a two-dimensional kernel polynomial method (KPM) [28–30]. In this approach, current–current correlation function $J(E,E')$ can thus be expanded as a series of Chebyshev polynomials $T_l(x)$:

$$\begin{aligned}J(E,E') &= \sum_{n,m}\big|\langle n|\hat{j}_x|m\rangle\big|^2\delta(E-E_n)\delta(E'-E_m) \\ &\approx \sum_{n,m}^{N_c}\frac{\mu_{nm}g_n g_m T_n(\tilde{E})T_m(\tilde{E}')}{b^2\pi^2\sqrt{(1-\tilde{E}^2)(1-\tilde{E}'^2)}}\end{aligned}$$

where coefficient $\mu_{nm} = Tr[\hat{j}_x T_n(\tilde{H})\hat{j}_x T_m(\tilde{H})]$. $b = E_{\max} - E_{\min}$ stands for band width and $\tilde{E} = E/b$ ($\tilde{H} = H/b$) is rescaled energy (Hamiltonian). $N_c = 2000$ is maximum number of polynomial used to expand the $J(E,E')$. g_n are Jackson kernel factors [28]. The Chebyshev polynomials $T_m(x)$ satisfy relation:

$$T_0(x) = 1, \qquad T_1(x) = x,$$
$$T_{m+1}(x) = 2xT_m(x) - T_{m-1}(x), \quad m > 0.$$

Moreover, with the help of KPM method, we can also obtain the density of states (DOS):

$$\rho(E) = -\frac{1}{\pi}Im\,G^R(E) \approx \sum_n^{N_c}\frac{\alpha_n g_n}{b\pi\sqrt{1-\tilde{E}^2}}T_n(\tilde{E}) \tag{3}$$

where $\alpha_n = Tr[T_n(\tilde{H})]$.

In order to illustrate the exotic transport properties near the Dirac point and reduce the finite-size effects, a very large lattice of more than one million sites is used. In this Letter, all results are performed on a lattice system $N_x \times N_y = 1600 \times 1600$. To show the results are robust against the finite-size effect, we also confirm the results in Fig. 1 unchanged up to a larger system size $N_x \times N_y = 4800 \times 4800$ (see below). In the calculations, the periodic boundary conditions are imposed. To calculate the trace in μ_{nm} efficiently, we also use stochastic evaluation method [31]. We have smoothed the curves by averaging over 500 disorder realizations to obtain averaged DOS and conductivity [32] (for system size 4800×4800, the results are only averaged over 50 disorder samples).

3. Coulomb impurities

The effects of Coulomb scattering impurities are introduced through random on-site energy $\epsilon_i = V(\mathbf{r}_i)$ in the second term of Eq. (1). In our model we assume that random potential is generated by N_i randomly distributed Coulomb impurities at position r_m whose potential with an interaction range of ξ:

$$V(\mathbf{r}_i) = \sum_{m=1}^{N_i}\frac{\alpha\hbar v_F}{|\mathbf{r}_i - \mathbf{r}_m|}e^{-\frac{|\mathbf{r}_i-\mathbf{r}_m|}{\xi}} \tag{4}$$

where $\hbar v_F = 3ta/2$ is the Fermi velocity and a is lattice constant. $\alpha = \frac{e^2}{\varepsilon\hbar v_F}$ is the effective fine structure constant used to characterize the Coulomb interaction in graphene and $\alpha \simeq 1$ when the graphene sheet is placed on a SiO_2 dielectric substrate [33]. ξ controls the interaction range of Coulomb scatters ($\xi \gg a$). We also assume that the impurity in the substrate is $d = 1$ nm away from the graphene plane. For a lattice of total N lattice sites, $n_{imp} = N_i/N$ is the impurity concentration.

To have a better knowledge about the random potential used in our calculations, Fig. 1(a) is the contour plot of a typical random potential generated by randomly distributed Coulomb impurity of interaction range $\xi = 20a$, much larger than the lattice constant so that random potential generated has a loop structure. Fig. 2(b) compares the total averaged DOS near the Dirac point for two different impurity concentrations of Coulomb scatters. The prominent dip at Dirac point for low impurities concentration ($n_{imp} = 3.8 \times 10^{11}$ cm^{-2}) is replaced by a smooth minimum at a larger value for the case of high impurity concentration ($n_{imp} = 3.8 \times 10^{12}$ cm^{-2}). The particular enhanced