

Scattering mechanisms and Boltzmann transport in graphene[☆]

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Abstract

Different scattering mechanisms in graphene are explored and conductivity is calculated within the Boltzmann transport theory. We provide results for short-range scattering using the random phase approximation for electron screening, as well as analytical expressions for the dependence of conductivity on the dielectric constant of the substrate. We further examine the effect of ripples on the transport using a surface roughness model developed for semiconductor heterostructures. We find that close to the Dirac point, $\sigma \sim n^\beta$, where $\beta = 1, 0, -2$ for Coulomb, short-range and surface roughness, respectively; implying that Coulomb scattering dominates over both short-range and surface roughness scattering at low density.

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1. Introduction

Over the last two years, there has been a proliferation in theoretical and experimental interest in graphene. Graphene is a two-dimensional sheet of carbon atoms arranged in a honey-comb lattice, or alternatively, a mono-atomic sheet of carbon that has been cleaved from bulk graphite onto a semiconductor substrate. Graphene has generated much excitement as theorists and experimentalists explore both the familiar and peculiar features of this newly discovered condensed matter system. Perhaps the most curious property of graphene was the “minimum conductivity” puzzle, where a naïve examination of experimental results would suggest that graphene had a finite conductivity even as the density of carriers vanishes. This “carrier-free” universal minimum conductivity has been the subject of much speculation in the recent literature. However, there is now mounting evidence [1,2] suggesting a more sensible alternative—charged impurities that are invariably present in the substrate create an inhomogeneous potential landscape [3]. At large external gate voltage

$V_g = n/\alpha \gg n_{\text{imp}}/\alpha$, where n_{imp} is the density of charged substrate impurities and α is related to the capacitance of the substrate, the potential fluctuations can be ignored, but at low density, they locally dope the graphene sheet breaking the system into puddles of electrons and holes. This spatial inhomogeneity has been directly observed in recent experiments [4]. We observe that the charged impurities therefore have a dual role: first, the induced graphene carrier density needs to be determined by the screened charged impurity potential, and second, the conductivity is determined by charged impurity scattering.

Unlike gapped 2D systems—where much of the same physics is at play—in graphene the electrons and holes are both conducting. So, whereas in semiconductor systems one might have a percolation transition between a conducting and insulating state [5], graphene transport, through this percolating network of electron and hole puddles, is a transition between two conducting states. One also finds that the system self-averages at length scales of the correlation length L_ξ , where $L_\xi \ll L$ and $L \sim 1 \mu\text{m}$ is the typical system size. This then allows us to calculate the transport properties using the *rms* carrier density n^* induced by the potential fluctuations (for details, see Ref. [6]). This mean-field theory is valid so long as n^* is sufficiently large so that the percolation transport is not

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critical—a condition we believe holds true for experiments currently being done on bulk graphene samples. Ref. [7] recently calculated the modification of the critical exponents due to the tunneling between the electron and hole puddles.

In the present work, we examine two other types of scattering that may be present in graphene, namely, short-range scattering (arising from defects or dislocations in the carbon lattice) and scattering from ripples. Both of these possible additional sources of scattering have been observed in recent surface probe measurements of graphene [8]. These experiments, however, also showed that graphene sheets are relatively defect free and the ripples, although present, are very small, where the average ripple height $\Delta = 1.9 \text{ \AA}$, while the in-plane correlation length $\xi = 320 \text{ \AA}$. These numbers cast serious doubt over whether the electron scattering of graphene ripples could have any observable effect on the transport properties of graphene. We observe that diffraction experiments performed on suspended graphene sheets show ripples of about the same height but with an order of magnitude smaller in-plane correlation length [9] further suggesting that the ripples of graphene on a substrate is largely determined by the roughness of that substrate.

For our purposes we reserve the term “long-range” scattering for Coulomb impurities and use the two phrases interchangeably. We consider all delta-correlated disorder (i.e. Gaussian white noise potentials) to be “short-range” scattering. Other definitions have been employed in the literature where white-noise disorder is sometimes described as long-range if it preserves the graphene valley degeneracy and short-range only if the disorder breaks this symmetry. In all of our discussion below we shall assume that both spin and valley degeneracy is always preserved.

Short-range scattering has been considered previously by many groups including Refs. [10–12] using various approximation schemes. Here, we present results for the screened short-range scattering using the random phase approximation (RPA) for electron screening [13] which allows us to extract the dependence of the conductivity on the interaction parameter r_s , which can be tuned by using substrates of different dielectric constants.

Coulomb scattering was considered by Ref. [12] in the completely screened approximation valid only in the limit $r_s \rightarrow \infty$ and numerically in Ref. [3,10,14]. To compare the different scattering mechanisms with each other and to provide the framework for our calculation, we reproduce here the analytic Coulomb scattering conductivity result that was previously reported in Ref. [6].

The scattering of electrons off ripples has been of recent theoretical interest. Despite the magnitude of the ripples being quite small, it is still believed to be responsible for the suppression of weak localization [15], as well as causing changes to the local chemical potential [16] and modification of the transport properties [17]. To provide an estimate for the contributions of static ripples to graphene transport properties, we use a surface roughness model that was

developed to model interface potential inhomogeneities in semiconductor heterojunction systems. We do not attempt here to provide a rigorous microscopic justification for applying this surface roughness model [18] to graphene, although given its success in modeling surface inhomogeneities in Si-MOSFETs, it provides a good starting point to model the matrix element for electrons scattering off the potential inhomogeneity caused by ripples. Whereas the formal validity of this model has yet to be established, we are persuaded that it captures at least qualitatively, many of the features of the effect of ripples on graphene transport.

2. Formalism

We calculate the Drude–Boltzmann conductivity (see Ref. [6] for a detailed discussion on the range of validity of this formalism) using $\sigma = (2e^2/h)E_F\tau$

$$\tau^{-1} = \frac{4E_F}{\pi\gamma^2} \int_0^1 d\eta \eta^2 \sqrt{1-\eta^2} \left| \frac{v(\eta)}{\varepsilon(\eta)} \right|^2, \quad (1)$$

where E_F is the Fermi energy, $\hbar^{-1}\gamma$ is the Fermi velocity and the momentum transfer $q = |\mathbf{k} - \mathbf{k}'| = 2k_F\eta$. The different types of impurities change the scattering potential $v(\eta)$ and screening is accounted for using the RPA dielectric function $\varepsilon(\eta)$ reported in Ref. [13]. For Coulomb scatterers, we use

$$v^C(\eta) = \frac{\sqrt{n_{\text{imp}}}\pi e^2}{\kappa k_F \eta}, \quad \sigma^C = \frac{2e^2}{h} \left(\frac{n}{n_{\text{imp}}} \right) \frac{1}{F_1(2r_s)}, \quad (2)$$

where $F_1(x)$ is given analytically by [6]

$$\frac{F_1(x)}{x^2} = \frac{\pi}{4} + 3x - \frac{3x^2\pi}{2} + x(3x^2 - 2) \frac{\arccos[1/x]}{\sqrt{x^2 - 1}}. \quad (3)$$

It is straightforward to generalize this formalism to calculate the conductivity of screened short-range scatterers. We have

$$v^S(\eta) = \sqrt{n_{\text{imp}}}u, \quad \sigma^S = \frac{4\pi e^2}{h} \frac{\gamma^2}{n_{\text{imp}}u^2} \frac{1}{F_2(2r_s)},$$

$$F_2(x) = \frac{\pi}{2} - \frac{16x}{3} + 40x^3 + 6\pi x^2 - 20\pi x^4 + 8x^2(5x^3 - 4x) \frac{\arccos[1/x]}{\sqrt{x^2 - 1}}. \quad (4)$$

This result demonstrates that screening does not change the carrier density independence of the conductivity arising from short-range scattering and further predicts how the conductivity depends on the dielectric constant of the substrate.

In similar fashion, we can solve the surface roughness model [18]. First to determine its importance near the Dirac point, we calculate the limit $n \rightarrow 0$ and find

$$\sigma^R(n \rightarrow 0) = \frac{e^2}{4\pi^2 h n^2 \Delta^2 \zeta^2 r_s^2} \frac{1}{F_2(2r_s)} \sim \frac{1}{n^2}. \quad (5)$$

Therefore, within this surface roughness model (and in a manner qualitatively similar to short-range scattering), this effect becomes unimportant at the lowest carrier densities and at low temperature. Since experimentally, the parameter $\sqrt{\pi n^* \xi} \gtrsim 3$, the limit $k_F \xi \gg 1$ is more realistic. An analytic result can be obtained in the unscreened limit (where we note that screening would only reduce the contribution from this effect). We find

$$\ell^R = \frac{\xi}{16\sqrt{\pi} k_F^2 r_s^2 \Delta^2},$$

$$\sigma^R(k_F \xi \gg 1) = \frac{e^2}{h} \frac{\xi}{8\sqrt{\pi} k_F \Delta^2 r_s^2}, \quad (6)$$

where the first equation suggests that the mean free path ℓ for surface roughness scattering is typically larger than the sample size. These results, naturally, strongly depend on how one models the surface roughness. Recently, an alternate model proposed by Ref. [17] suggested that in some special circumstances ripples can mimic Coulomb scatterers, although their phonon model additionally predicts strong temperature dependence (above a certain quenching temperature of about 100 K)—an effect that has not been observed in the experiments. We do not believe that the ripples in graphene are playing an important direct quantitative role in determining the carrier mobility in currently available samples, but rather scattering due to unintentional charged impurities is the dominant scattering mechanism in graphene.

In Fig. 1 we show the effect of changing substrate dielectric constant on graphene transport properties. The blue circles show the experimental data of Ref. [2] for a high mobility sample, and the red solid curve ($\kappa = 3.9$) uses

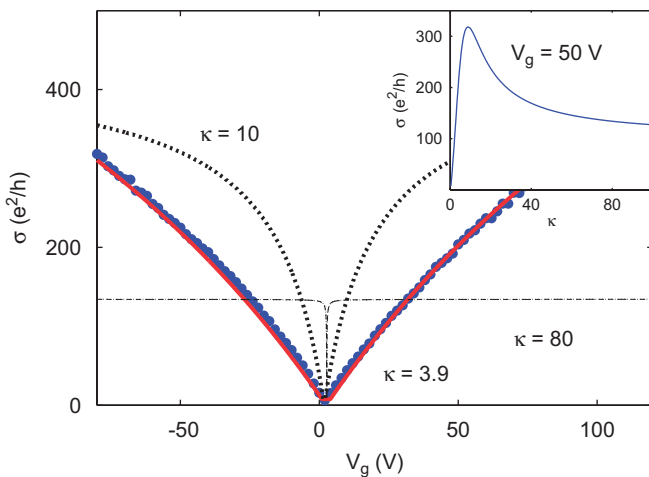


Fig. 1. This shows the dependence of conductivity on substrate dielectric constant κ . Filled blue circles show experimental data of Ref. [2]. Solid, dashed and broken lines show theoretical results for $\kappa = 3.9, 10, 80$, respectively. For large κ short-range scattering dominates while for small κ Coulomb scattering dominates. The inset shows that for a fixed gate voltage, the conductivity has a non-monotonic dependence on κ which is a consequence of the competition between short-range and long-range scattering.

the experimentally reported values in that paper for the undetermined parameters in our theory. A single fit parameter is still necessary to obtain the overall scale of the short-range impurities. Theoretical predictions for different dielectric constants are also shown. For $\kappa \lesssim 5$, Coulomb scattering dominates (as is the case in most current experimental samples), while for larger dielectric constant, Coulomb scattering is more strongly screened making short-range scattering more dominant (see broken curve with $\kappa = 80$). For intermediate values of dielectric constant, we have a crossover from low-density Coulomb scattering dominated behavior to high-density short-range scattering dominated (see dashed curve with $\kappa = 10$).

3. Discussion and conclusion

We have examined three different sources of scattering in graphene and treated them in the RPA-Boltzmann regime which we believe provides the basic formalism to understand current graphene experiments. This formalism strongly indicates that close to the Dirac point, the transport properties are dominated by Coulomb impurity scattering.

The basic picture is quite intuitive. As described above, within the RPA-Boltzmann formalism, charged impurities in the substrate provide a contribution to the conductivity that is proportional to the number of carriers in the graphene sheet. Additionally, these same charged impurities generate potential fluctuations that are screened by any carriers in the graphene sheet. A self-consistent procedure [6] is used to determine the residual carriers that contribute to Boltzmann conductivity even as the external gate voltage is tuned through the duality point where the majority of carriers changes from electrons to holes. This mean-field residual carrier density n^* provides for a minimum conductivity plateau and is in quantitative agreement with recent experimental data [1,2]. In this context, the current work demonstrates that other scattering mechanisms do not alter this picture. Additionally, this work makes several predictions that can be tested experimentally if one is able to change the substrate onto which graphene has been cleaved. Experiments have already been performed on graphene sandwiched between various kinds of plastics using a transfer printing method [19] and experiments in the near future will certainly test the predictions we make in this work.

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