Impurity scattering induced carrier transport in twisted bilayer graphene

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We theoretically calculate the impurity-scattering induced resistivity of twisted bilayer graphene at low twist angles where the graphene Fermi velocity is strongly suppressed. We consider, as a function of carrier density, twist angle, and temperature, both long-ranged Coulomb scattering and short-ranged defect scattering within a Boltzmann theory relaxation time approach. For experimentally relevant disorder, impurity scattering contributes a resistivity comparable to (much larger than) the phonon scattering contribution at high (low) temperatures. Decreasing twist angle leads to larger resistivity, and in general, the resistivity increases (decreases) with increasing temperature (carrier density). Inclusion of the van Hove singularity in the theory leads to a strong increase in the resistivity at higher densities, where the chemical potential is close to a van Hove singularity, leading to an apparent density-dependent plateau type structure in the resistivity, which has been observed in recent transport experiments. We also show that the Matthiessen’s rule is strongly violated in twisted bilayer graphene at low twist angles.

**Introduction** – Electronic properties, particularly ohmic transport properties, of twisted bilayer graphene (TBLG) are of great current interest because of the seminal experimental findings by Cao et al. at MIT that TBLG has intriguing low-temperature density- and temperature-dependent transport behavior. In particular, both superconducting and insulating ground states seem to exist in TBLG at various carrier densities and low twist angles.$^{1-4}$ The resultant density-temperature-twist angle dependent TBLG phase diagram is rich and complex, and is being actively studied in many laboratories. Although there are many proposed theories for TBLG ground states, there is no consensus yet on the nature of the superconducting (S) or insulating (I) ground states.

Our theoretical work is on electronic transport above the ground state, i.e., at elevated temperatures (much larger than the corresponding gap defining the S or I phase) where superconducting or insulating behavior is suppressed and the system behaves like an effective metal, as found experimentally.$^{5,6}$ The issue we address is how disorder in TBLG samples affects the ohmic transport properties, assuming that the system can be considered to be an effective 2D metal with a finite carrier density. Effect of phonon scattering on TBLG ‘metallic’ transport has recently been considered in the literature,$^{7-10}$ so we focus on the effect of impurity scattering. One motivation for our considering impurity scattering effects is the fact that disorder is known to be the most important resistive scattering source in regular (i.e., untwisted) graphene up to room temperatures because the typical electron-phonon coupling in regular graphene is weak. It has been argued in Ref. $^2$ that the strong suppression in the TBLG Fermi velocity at low twist angles leads to a giant enhancement in the effective electron-phonon coupling, causing a large contribution to the phonon-induced temperature-dependent resistivity. In the current work, we address the issue of the effect of TBLG Fermi velocity suppression on impurity scattering-induced graphene resistivity. In addition, we investigate the extent to which the Matthiessen’s rule applies to TBLG transport at finite temperatures by taking into account resistive scattering from both phonons and impurities. We find that Matthiessen’s rule is strongly violated in TBLG at low twist angles leading to the actual resistivity being 100% (or more) larger than the sum of the individual impurity and phonon resistivities.

**Theory, Model, and Results** – Detailed theories for impurity scattering effects in graphene are already available in the literature,$^{8-10}$ which would not be reproduced here since we use the standard theory$^{8-10}$ involving Boltzmann equation and relaxation time approximation within the leading order scattering approximation. The main question in calculating the impurity resistivity is modeling the impurity scattering potential and the TBLG electronic structure. Unfortunately, neither is well-established at this early developing stage of the subject, and in fact, even in regular untwisted graphene, settling the precise nature of disorder scattering limited resistivity took some time.$^{8-15}$

The nature of the dominant impurity scattering in TBLG is not known, and the precise TBLG electronic structure is also unknown. In particular, it is believed that there is some twist angle fluctuation related disorder in TBLG, but there is no available quantitative information on this disorder. It is reasonable to assume that disorder effects existing in regular graphene, random charged impurities and point defects, are also present in TBLG since TBLGs are formed by two monolayers of regular graphene. Following the well-established disorder model in untwisted graphene, we assume that TBLG has two types of disorder: long-range disorder arising from random charged impurities and short-range disorder arising neutral impurities and defects. We subsume the unknown twist angle fluctuation disorder as contribut-
ing to the short-range disorder part of our model. Our impurity model thus has two unknown independent parameters corresponding to the density of random charged impurities and the strength of the short range disorder.

The dominant physics of the TBLG electronic structure affecting transport properties is the twist angle dependent flattening of the moiré superlattice bands operational in the system. This band flattening leads to a strong suppression of the graphene Fermi velocity with decreasing twist angle. Following Ref. [16], we include in the theory the band flattening effect through a modified Fermi velocity arising from the moiré superlattice structure of the system. The dependence of the Fermi velocity on the twist angle is already given in Ref. [7], and not reproduced here. We show our results as a function of the TBLG Fermi velocity which we take as a variable – the dependence of this reduced Fermi velocity on the twist angle follows the electronic structure model introduced in Ref. [10] and the corresponding Fermi velocity \( v_F \) as a function of the twist angle is given in [7]. More sophisticated electronic structure can be incorporated in the theory at the considerable price of all analytical transparency being lost since all matrix elements must be calculated numerically, which would be quite demanding for a finite temperature transport calculation of interest here. Also, using complicated electronic structure for transport calculations may be an unnecessary overkill at this stage of development of the subject since the precise nature and the quantitative details of the underlying disorder in TBLG are unknown right now. More importantly, the electronic structure of the TBLG moiré superlattice is far from being accurately known with considerable sample to sample variations. These variations could arise from strain relaxation in the TBLG and/or from twist angle fluctuations or from other unknown sources. Therefore, it makes sense in this early stage of the subject to use a minimal model for the TBLG electronic structure, which obviously is the incorporation of the flatband induced twist angle dependent Fermi velocity suppression in the theory. At higher carrier density, as the chemical potential approaches a van Hove singularity (vHS) as well below the TBLG Fermi level or chemical potential is well below any vHS, and neglecting the vHS effect is a valid approximation. The resistivity \( \rho = 1/\sigma \), where the conductivity \( \sigma \) is given by

\[
\sigma(n, T) = \frac{e^2 g v_F k_F}{\hbar} \langle \tau \rangle,
\]

where \( g \) is the total degeneracy, \( k_F \) is the Fermi wave vector, and \( \langle \tau \rangle \) is the relaxation time averaged over energy. For impurity scattering we consider the screened long range Coulomb disorder and unscreened short range disorder. The impurity scattering of long range disorder is determined by the impurity charge density \( n_i \) and the scattering of short range disorder is determined by the parameter \( n_d V_0^2 \), where \( n_d \) is the impurity density and \( V_0 \) is the strength of the potential.

In order to find the total resistivity at finite temperatures we have to calculate the energy averaged transport relaxation time \( \langle \tau \rangle \) after adding the individual scattering rates due to impurities (i) and acoustic phonons (ph), i.e., \( \tau^{-1}_{\text{tot}} = \tau^{-1}_{\text{imp}} + \tau^{-1}_{\text{ph}} \), which deviates from adding the averaged individual scattering rate, i.e., \( \langle \tau^{-1}_{\text{imp}} \rangle = \langle \tau^{-1}_{\text{ph}} \rangle \). The other important temperature effect of scattering times in our model comes from temperature dependent screening in the screened long range disorder. We consider the temperature dependent screening (or dielectric function), i.e., \( \epsilon(q, T) = 1 - v(q) / \Pi(q, T) \), where \( v(q) = 2 \pi e^2 / \kappa q \) is the electron-electron interaction with a background dielectric constant \( \kappa \) and \( \Pi(q, T) \) is the irreducible finite-temperature polarizability function. For phonon scattering, we follow Refs. [13,14], which we do not reproduce here. Note that there are a number of variables and system parameters determining the TBLG resistivity: carrier density (determining \( k_F, E_F \), etc.), twist angle (determining electronic structure and particularly, \( v_F \), disorder strength (characterized by the parameters for long- and short-range impurities), phonon scattering strength (which, following Ref. [7], we take to be the deformation potential coupling appropriate for TBLG).

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First, we discuss the situation without considering vHS effects, which is valid at relatively low carrier densities \( n < 2 \times 10^{12} \, \text{cm}^{-2} \) near the Dirac point. For doping densities not too far from the Dirac point (for less than ‘quarter filling’ either on the electron or the hole side), the TBLG Fermi level or chemical potential is well below any vHS, and neglecting the vHS effect is a valid approximation. The resistivity \( \rho = 1/\sigma \), where the conductivity \( \sigma \) is given by

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FIG. 2: (a) Calculated resistivity with both long range charged disorder and short range neutral disorder as a function of $v_F$ for a fixed carrier density $n = 1.2 \times 10^{12} \text{cm}^{-2}$. Here the charged impurity density $n_i = 3 \times 10^{10} \text{cm}^{-2}$ and the neutral disorder strength $n_d V_0^2 = 0.53 \text{eV} \AA^2$ are used. (b) The resistivity as a function of density for several $v_F$ with the same disorder parameters as (a). (c) The temperature dependent resistivity, $\rho(T)/\rho(0)$ where $\rho(0)$ is the resistivity at $T = 0$, as a function of $T/T_F$ for several $v_F$ with the same disorder parameters as (a). Twist angles corresponding to $v_F = 10^8$, $10^7$, $10^6 \text{cm/s}$ are $\theta = 25^\circ$, $1.24^\circ$, $1.06^\circ$, respectively.

The neutral disorder strength $n_d V_0^2 = 0.53 \text{eV} \AA^2$ are used. For a fixed Fermi velocity $v_F$, the charged impurity density $n_i = 3 \times 10^{10} \text{cm}^{-2}$ and the neutral disorder strength $n_d V_0^2 = 0.53 \text{eV} \AA^2$. The total scattering rate $\tau = \tau_{\text{tot}}$ is shown as a function of Fermi velocity $v_F$ for several $v_F$ with the same disorder parameters as (a). Twist angles corresponding to $v_F = 10^8$, $10^7$, $10^6 \text{cm/s}$ are $\theta = 25^\circ$, $1.24^\circ$, $1.06^\circ$, respectively.

The Matthiessen’s rule on the additivity of resistivities for different scattering mechanisms will not hold in most cases at finite temperatures. In general, the energy-averaged scattering rates do not add because the energy averaging is for $\tau$ rather than for $1/\tau$. We show that the

\[ \sigma_0(v_F) \sim \text{const. for } v_F \to 0 \left( \theta \to \text{magic angle} \right) \]
\[ \sim v_F^2 \quad \text{for } v_F \to \infty, \quad (2) \]

For long range disorder

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Matthiessen rule, i.e., $\rho_{\text{tot}} = \rho_{\text{ph}} + \rho_i$, where $\rho_{\text{tot}}$ is the total resistivity contributed by impurities $\rho_i$ and phonons $\rho_{\text{ph}}$, is simply not valid in the small angle twisted bilayer graphene.

In Fig. 3 we show the calculated resistivity as a function of temperature for various Fermi velocities (twist angles), (a) $v_F = 10^7 \text{ cm/s (}\theta = 1.24\degree\text{)}$, (b) $v_F = 5 \times 10^6 \text{ cm/s (}\theta = 1.14\degree\text{)}$, (c) $v_F = 2.5 \times 10^6 \text{ cm/s (}\theta = 1.09\degree\text{)}$, and (d) $v_F = 2.1 \times 10^6 \text{ cm/s (}\theta = 1.08\degree\text{)}$, considering two types of impurity scattering (screened long range impurity and unscreened short range impurity) and phonon scattering. The screened charged impurity density $n_i = 5 \times 10^{10} \text{ cm}^{-2}$ and the short range disorder strength $n_d\sqrt{V_0} = 0.72 \text{ eV}^2\text{nm}^2$ are used. The deformation potential $D = 15 \text{ eV}$ is used for the acoustic phonon scattering throughout this paper. By calculating the total resistivity arising from impurity scattering $\tau_i$ and phonon scattering $\tau_{\text{ph}}$ we clearly show that $\rho_{\text{tot}} > \rho_{\text{ph}} + \rho_i$ for lower Fermi velocities. It is obvious from our results in Fig. 3 that the Matthiessen’s rule may fail badly for TBLG at low twist angles where the Fermi velocity (i.e., the twist angle) is small. However, the differences are smaller for larger Fermi velocities (or larger angle TBLG).

Inclusion of van Hove singularity – The above results are for low chemical potential with typical doping densities being around the Dirac point ($< 2 \times 10^{12} \text{ cm}^{-2}$) so that the TBLG is less than quarter-filled. At higher densities, as a vHS is approached, the theory must include the vHS in some manner. Here, we demonstrate the vHS effect simply by considering various model density of states (DOS) as described below. Our theory of transport in the presence of vHS using these simple model DOS should be taken as a zeroth order impurity scattering theory establishing the qualitative importance of vHS in determining TBLG transport at higher doping densities. We use the density of states having a logarithmic van Hove singularity at a density $n_0$ such as

$$D(n) = D_0 \sqrt{\pi n_0} \left[1 + \alpha \ln(1 - n/n_0)\right], \quad (4)$$

where $D_0 = \sqrt{g n_0 \pi / \hbar v_F}$ and $\alpha$ is a parameter which controls the strength of the singularity of DOS at $n = n_0$.

In Fig. 4 the resistivity, which is calculated with the density of states corresponding to Eq. (4), is shown as a function of carrier density. In Fig. 4(a) we show the density of states for three different $\alpha=0, 1, 3$ and for $n_0 = 10^{12} \text{ cm}^{-2}$. Fig. 4(b) shows the calculated resistivity for different $\alpha$ with a fixed charged impurity density $n_i = 5 \times 10^{10} \text{ cm}^{-2}$ and a fixed neutral disorder strength $n_d\sqrt{V_0} = 10 \text{ eV}^2\text{A}^2$. A resistivity peak appears at the singular point of DOS and the strength of the peak is strongly correlated to the singular feature of DOS. The resistivity for different combinations of charged impurity density and neutral disorder strength is shown in Fig. 4(c) and (d) for $\alpha = 3$. The calculated resistivity is significantly (weakly) affected by long range disorder at low carrier densities (near the singular point of DOS). However, as shown in Fig. 4(d) the calculated resistivity is greatly (significantly) affected by short range disorder at low carrier densities (near the singular point of DOS).
In Fig. 5 the resistivity is calculated with the DOS having two singularities at \( n_0 \) and \( 2n_0 \), i.e.,

\[
D(n) = D_0 \sqrt{n/n_0} \left\{ 1 + \frac{\alpha}{2} \ln \left[ \left(1 - \frac{n}{n_0}\right)^2 + \eta \right] + \frac{\beta}{2} \ln \left[ \left(1 - \frac{n}{2n_0}\right)^2 + \eta \right] \right\}, \tag{5}
\]

where \( \alpha \) and \( \beta \) are constants determining the strength of the singularities and \( \eta \) is introduced as a broadening to suppress the singular behaviors of DOS. Figs. 5(a) and (b) show the calculated resistivity for different combinations of charged disorder and neutral disorder with \( \alpha = 1 \) and \( \beta = 2 \), where the strength of the second peak in DOS is two times larger than that of the first peak. The resistivity is also shown in Figs. 5(c)(d) for \( \alpha = \beta = 2 \). It is clear from these results that vHS have profound effects on TBLG transport. In particular, Fig. 5 shows that the resistivity in the presence of multiple vHS manifests a plateau-like almost-constant structure in between the vHS-induced resistivity maxima. Such peak and plateau type resistivity in between various commensurate filling has actually been observed as a function of doping density in Ref. [8], and we believe that vHS is the physical mechanism underlying these resistivity plateaus.

**Conclusion** – We have theoretically calculated impurity scattering induced TBLG transport showing the profound effects of the velocity suppression and van Hove singularity in the moiré system. In particular, the Matthiessen’s rule is strongly violated in TBLG at small twist angles (where \( v_F \) is low) and the presence of vHS produces resistivity peaks with plateau-like density-dependent resistivity in between the peaks.

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