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Theory of carrier transport in bilayer graphene

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We develop a theory for density, disorder, and temperature-dependent electrical conductivity of bilayer graphene in the presence of long-range charged impurity scattering and short-range defect scattering, establishing that both contribute significantly to determining bilayer transport properties. We find that although strong screening properties of bilayer graphene lead to qualitative differences with the corresponding single-layer situation, both systems exhibit the approximately linearly density-dependent conductivity at high density and the minimum conductivity behavior around the charge neutrality point due to the formation of inhomogeneous electron-hole puddles. The importance of short-range disorder in determining bilayer conductivity is a qualitative finding of our work.

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Ever since the discovery of graphene,[1] its transport properties as functions of carrier density and temperature have been of key fundamental and technological interest. The fundamental interest arises from the unique linear massless chiral Dirac dispersion of electrons (holes) in the graphene conduction (valence) band with the system being a zero-gap semiconductor which on doping (or external-field-induced gating) changes its character continuously from being an "electron-metal" to a "hole-metal" as it goes through the charge neutral Dirac point. Unique transport properties of massless, gapless, and chiral Dirac particles in two-dimensional (2D) single-layer graphene (SLG) as functions of their density and temperature have attracted a great deal of experimental and theoretical attention over the last few years.

More recently, however, carrier transport in 2D bilayer graphene (BLG) has attracted considerable attention.[2–4] In BLG, the carriers tunnel quantum mechanically between the two layers leading to a modified band dispersion which is approximately parabolic with an effective mass of about $0.033m_e$.[4] BLG transport thus involves dynamics of chiral, parabolic dispersion carriers in the zero band-gap situation in contrast to the chiral, linear-dispersion Dirac carrier system for SLG. Among the characteristic observed features of BLG carrier transport to be explained theoretically are a substantially suppressed BLG mobility with respect to the SLG mobility, a lower value of the minimum conductivity around the charge neutrality point compared with the SLG situation, and an enhanced temperature dependence of conductivity. In spite of the much lower observed BLG mobility compared with the SLG mobility, the density dependence of BLG conductivity seems to manifest the same linear behavior as seen in the SLG transport. In the current work, we investigate the effect of chiral parabolic band dispersion on graphene diffusive transport properties to see if we can understand the observed BLG transport behavior as well as to compare and contrast with the corresponding chiral linear SLG band-dispersion results.

In this Rapid Communication we develop the quantitative theory for BLG carrier transport in the presence of random charged impurity (i.e., long-range Coulomb[5]) and short-range defect scattering.[6] Our goal here is to develop a theory capable of making quantitative predictions about the temperature and density-dependent BLG conductivity both at high-carrier density and at the charge neutrality point at low-carrier density. We make the reasonable assumption that the actual BLG scattering mechanisms cannot be radically different from the ones operational in SLG (Refs. 7 and 8) since both systems are made by identical exfoliation techniques. As such we consider the presence of long-range charged impurity and short-range defect scattering as the resistive mechanisms in our theory. In addition, the experimentally measured BLG conductivity is large enough ($\sigma > 3e^2/h$) so that the typical "$k_F l$" values are in the range of 6–200 implying the validity of the semiclassical Boltzmann transport theory with the Born approximation for scattering. Quantum (as well as higher-order scattering) corrections to our theory should be smaller by factors of $O[(k_F l)^{-2}]$ or larger and can thus be neglected for the diffusive transport properties.

We start by providing a qualitative conceptual discussion of BLG transport properties vis a vis SLG transport. Because of the linear (SLG) versus quadratic (BLG) energy dispersion in the two cases, the density of states is linear (constant) in SLG (BLG), leading to very distinct screening behavior in the two cases:[9,10] $q_{TF}^{\mathrm{SLG}} \propto k_F$; $q_{TF}^{\mathrm{BLG}} \propto k_F^0 =$ constant, where q_{TF} is the long wavelength Thomas-Fermi screening wave vector and $k_F \propto \sqrt{n}$ is the Fermi wave vector (with n as the tunable 2D carrier density). Therefore, the screened Coulomb impurity potential, $u_i(q)$, behaves very differently in the two systems: $u_i^{\mathrm{SLG}}(q) \sim k_F^{-1}$; $u_i^{\mathrm{BLG}} \sim (q_{TF}+k_F)^{-1}$, where $q_{TF} \equiv q_{TF}^{\mathrm{BLG}} = (4me^2)/(\kappa\hbar^2) \approx 10^7$ cm^{-1}, where κ is the background environmental dielectric constant. Thus, the nature of screened Coulomb scattering is qualitatively different in the two systems—in fact, the screened Coulomb disorder in the SLG behaves as unscreened Coulomb interaction [i.e., $v(q) \sim 1/q$] (Ref. 9) whereas the screened Coulomb disorder in the BLG behaves similar to the 2D screened Coulomb interaction although there are some differences.[10] It is, therefore, quite puzzling that experimentally the two systems have very similar carrier-transport properties.[2,3] Away from the charge neutral point, CNP, ($n=0$), both manifest a conductivity, σ, approximately proportional to n, whereas for $n \sim 0$ the conductivity is approximately constant, forming the much-discussed graphene minimum conductivity plateau in both

cases. The striking similarity of the experimentally observed density-dependent conductivity $\sigma(n)$ in the two systems presents a serious challenge to transport theories since the nature of screened Coulomb disorder in the two systems is fundamentally different.

In this Rapid Communication we propose that BLG carrier transport is controlled almost equally by two distinct and independent physical scattering mechanisms: screened Coulomb disorder due to random charged impurities in the environment and a short-range disorder which is important throughout (i.e., all the way from the CNP manifesting the plateaulike minimum conductivity behavior to the high-density conductivity increasing linearly with carrier density). We find that neither pure Coulomb disorder nor pure short-range disorder by itself can explain *both* the density and the T dependence of the experimentally observed BLG conductivity behavior. We emphasize that the actual amount of Coulomb and short-range disorder we need to qualitatively and semiquantitatively explain the existing BLG transport data is comparable to that already used in understanding the SLG transport properties, and as such, there is no arbitrary data fitting procedure in our theory.

The density- and temperature-dependent BLG conductivity is given within the Boltzmann transport theory by $\sigma = (e^2/m)\int d\epsilon D(\epsilon)\epsilon\tau(\epsilon)(-\partial f/\partial\epsilon)$, where $D(\epsilon)$, $\tau(\epsilon)$, and f are, respectively, the energy-dependent density of states, the transport relaxation time (which depends explicitly on the scattering mechanism), and the (finite-T) Fermi distribution function. τ is given by

$$\frac{1}{\tau(\epsilon_{s\mathbf{k}})} = \frac{2\pi n_0}{\hbar}\int \frac{d^2k'}{(2\pi)^2}|\langle V_{s\mathbf{k},s\mathbf{k}'}\rangle|^2 g(\theta_{\mathbf{k}\mathbf{k}'}) \times [1-\cos\,\theta_{\mathbf{k}\mathbf{k}'}]\delta(\epsilon_{s\mathbf{k}}-\epsilon_{s\mathbf{k}'}), \quad (1)$$

where $\epsilon_{s\mathbf{k}} = s\hbar^2k^2/2m$ is the carrier energy for the spin/pseudospin state "s" and 2D wave vector $\mathbf{k}$, $\langle V_{s\mathbf{k},s\mathbf{k}'}\rangle$ is the matrix element of the appropriate disorder potential, $g(\theta) = [1+\cos(2\theta)]/2$ is a wave function form factor associated with the chiral nature of BLG (and is determined by its band structure). In Eq. (1), n_0 is the appropriate 2D areal concentration of the impurity centers giving rise to the random disorder potential V. We consider two different kinds of disorder scattering: (i) screened Coulomb disorder u_i for which $n_0|\langle V_{s\mathbf{k},s\mathbf{k}'}\rangle|^2 = n_i|u_i|^2 = n_i|v_i(q)/\epsilon(q)|^2$ and (ii) short-range disorder V_0 for which $n_0|\langle V_{s\mathbf{k},s\mathbf{k}'}\rangle|^2 = n_d V_0^2$. Here $q \equiv |\mathbf{k}-\mathbf{k}'|$, $v_i(q) = (2\pi e^2/\kappa q)$ is the 2D Coulomb potential, and V_0 a constant short-range (i.e., a δ function in real space) potential. (Note that we use n_i to denote the charged impurity density.) The dielectric screening function $\epsilon(q)$ entering the effective screened Coulomb disorder, which depends on both q and T, was calculated in Ref. 10 at $T=0$, and we have now generalized it to $T\neq 0$ as shown in Fig. 1. Note that BLG screening peaks at $2k_F$ which is also the important scattering wave vector due to the form factor g in Eq. (1).

It is straightforward to calculate the analytical density dependence (for $T/T_F \ll 1$) of BLG (SLG) conductivity from the above formulas: $\sigma(n)\sim n^2(n)$ for unscreened Coulomb disorder; $\sigma(n)\sim n(n)$ for overscreened Coulomb disorder; $\sigma(n)\sim n^\alpha(n)$ and $1<\alpha<2$ for screened Coulomb disorder;

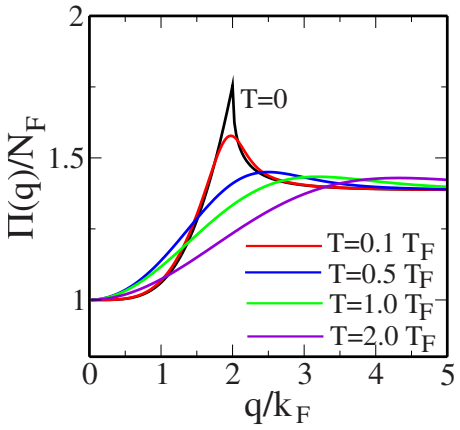

FIG. 1. (Color online) The wave-vector-dependent 2D BLG polarizability Π (in units of the density of states at the Fermi level N_F) for different values of $T/T_F = 0, 0.1, 0.5, 1.0, 2.0$, where $T_F = E_F/k_B$ is the Fermi temperature ($T_F \approx 831$ K for $n = 10^{12}$ cm^{-2}) and the dielectric function is given by $\epsilon = 1 + v_c\Pi$ where v_c is the 2D Coulomb interaction. The ordinate can be taken as a measure of the strength of BLG screening in units of Thomas-Fermi screening constant $q_{TF} \approx 10^7$ cm^{-1}.

$\sigma(n)\sim n$ (constant) for short-range disorder. We emphasize that $\alpha(n)$ is a density-dependent exponent which varies slowly changing from 1 at low density to 2 at high density—in the BLG experimental density range $\alpha \approx 1.2$. Increasing temperature, in general, suppresses screening, leading to a slight enhancement of the exponent α. The qualitative difference between BLG and SLG is that short-range scattering contributes substantially to the BLG resistivity whereas it does not for SLG resistivity, thus leading to a suppressed mobility in BLG compared with SLG mobility.

It is obvious from the above discussion that Coulomb disorder by itself cannot explain the experimentally observed linear density dependence of $\sigma(n)$ in BLG. By contrast, the SLG conductivity for Coulomb disorder, either screened or unscreened, follows the linear $\sigma(n)\sim n$ behavior whereas the short-range disorder leads to a density-independent $\sigma(n)\sim n^0$ behavior. Thus, the carrier-transport physics is fundamentally and qualitatively different in SLG and BLG: in SLG carrier transport is *always* dominated by Coulomb disorder except at extreme high densities, whereas in BLG the short-range disorder is always asymptotically more important than Coulomb disorder since the exponent $\alpha > 1$.

In Fig. 2 we present our full numerically calculated BLG conductivity as a function of n for reasonable representative values of disorder strength. The results shown in Fig. 2 are in good agreement with recent experimental results[2,3] but we do not make any attempt to obtain exact quantitative agreement since the experimental results show substantial sample-to-sample variations.[11] Instead we discuss the salient qualitative features of our results: (i) the calculated density dependence is approximately linear over a wide density range as seen experimentally; (ii) the temperature dependence is very weak at higher densities as observed in recent experiments;[2] (iii) at low densities, where T/T_F is not too small, there is a strong insulating-type T dependence arising from the thermal excitation of carriers (which is exponentially suppressed at

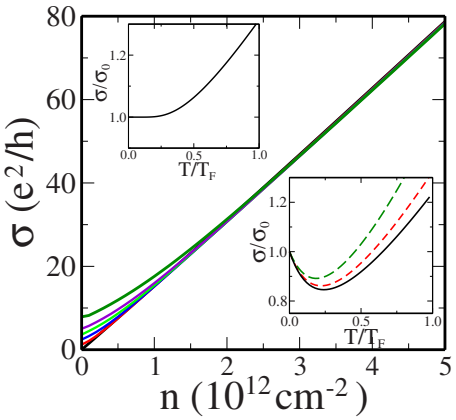

FIG. 2. (Color online) (a) Density dependence of BLG conductivity for different temperatures, $T=0,50,100,150,200,300$ K (from bottom to top), $n_i=10^{11}$ cm^{-2} and $n_d V_0^2=2.0$(eV Å)^2. Top inset shows σ as a function of T in presence of short-range disorder. The scaled conductivity applies for all densities. Bottom inset shows σ as a function of T in presence of screened Coulomb disorder for different densities $n=5,10,30\times10^{11}$ cm^{-2} (from bottom to top). Here $\sigma_0=\sigma(T=0)$.

higher densities) and energy averaging, as observed experimentally;[2] and (iv) when the dimensionless temperature is very small ($T/T_F \ll 1$) our theory necessarily predicts (see lower inset of Fig. 2) a weak linear-in T metallic T dependence arising from the temperature dependence of the screened charge impurity scattering, i.e., the thermal suppression of the $2k_F$ peak associated with backscattering in Fig. 1—this effect is enhanced in BLG due to the importance of backscattering whereas it is suppressed in SLG. By contrast, for the short-range disorder σ always increases with T, as shown in the upper inset of Fig. 2.

While the calculations for Fig. 2 are all carried out for graphene on SiO_2 substrate (corresponding to $\kappa \approx 2.5$), we have carried out detailed calculations of $\sigma(n,T,\kappa)$ as a function of the effective background dielectric constant (not shown) since screened Coulomb disorder should manifest a strong dependence on κ. Our calculations show the κ dependence of the net conductivity to be almost unobservable—for example, covering BLG on SiO_2 with ice, thus changing κ from 2.5 to 3.5, would only increase the conductivity by 1%, for $n_i=10^{11}$ cm^{-2}, and 10%, for $n_i=10^{12}$ cm^{-2}.

The Boltzmann theory presented so far assumes a completely homogeneous carrier-density landscape over the BLG sample and leads to $\sigma(T=0)=0$ at the CNP ($n=0$). It is, however, well known that SLG breaks up into an inhomogeneous landscape of electron-hole puddles around the CNP.[12–14] We expect the same physics of electron-hole puddles to dominate the BLG properties around the CNP, and this will give rise to a finite "minimum conductivity," $\sigma_{\min} \equiv \sigma(n=0)$ even in the limit $T \to 0$. We have investigated the properties of BLG puddle formation by calculating the ground state of the BLG in the presence of random charged impurities solving the density-functional equations within a local density approximation.[13] Using the resultant ground-state-density landscape $n(\mathbf{r})$ with $n \equiv \langle n(\mathbf{r}) \rangle_{\mathbf{r}}$ and averaging over disorder realizations we have then calculated the BLG

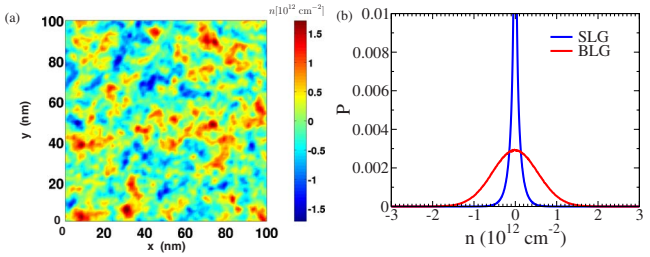

FIG. 3. (Color online) (a) $n(\mathbf{r})$ of BLG at the CNP for a single disorder realization with $n_i=10^{11}$ cm^{-2} and $d=1$ nm. (b) Disorder averaged $P(n)$, at the CNP for BLG (SLG) red and broad curve (blue and narrow curve) for $n_i=10^{11}$ cm^{-2} and $d=1$ nm. For SLG $P(n=0)\approx 0.1$, out of scale. The corresponding $n_{\rm rms}$ is 5.5×10^{11} cm^{-2} for BLG and 1.2×10^{11} cm^{-2} for SLG.

transport properties using the effective medium theory, EMT.[15] The details of the calculations will be presented elsewhere, here we present the realistic conductivity results in the puddle dominated regime obtained using our EMT.

In Fig. 3(a) we show our calculated zero-density puddle structure for the BLG for a single disorder realization with $n_i=10^{11}$ cm^{-2}. We note that by neglecting the disorder-induced inhomogeneities BLG (SLG) would have perfect (vanishing) linear screening properties as $n \to 0$, whereas the strong carrier-density fluctuations and associated electron-hole puddle structure induced by the charged impurities close to the CNP are qualitatively very similar in BLG and SLG. The linear (SLG) versus parabolic (BLG) carrier dispersion has the quantitative effect of modifying the form of the probability distribution $P(n)$ and make it much wider in BLG than in SLG, as shown in Fig. 3(b).

Finally in Fig. 4 we show $\sigma(n)$ for BLG for several values of T, taking into account the inhomogeneity of the puddles. These results are calculated numerically through the EMT by combining the density-functional electronic-structure calculation with the full Boltzmann transport theory. At high density ($\gg n_i$), the theory gives the same results as that obtained from the Boltzmann theory in the homogeneous case (i.e., Fig. 2) but at low densities there are significant deviations.

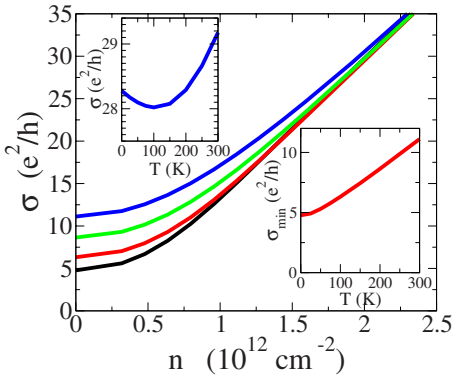

FIG. 4. (Color online) Conductivity as a function of n obtained using the EMT for $n_i=10^{11}$ cm^{-2}, $n_d V_0^2=2$(eV Å)^2 and several values of T, from top to bottom: $T=300,200,100,0$. From the slope for $n>10^{12}$ cm^{-2} for $T=0$ we extract a mobility of 4000 cm^2/Vs. In the lower (upper) inset $\sigma_{\min}$ [$\sigma(n=1.9\times10^{12}$ cm^{-2})] as a function of T for the same values of disorder strengths.

For example, we now get a well-defined finite $\sigma_{\min}$ even at $T=0$. We show the T dependence of the conductivity for $n=0$ and $n \gg n_i$ in the insets obtaining good agreement with the experimental finding[2,3] of a strong insulating T dependence of $\sigma_{\min}$. Our calculated $\sigma_{\min}$ depends weakly on n_i with no universally discernible functional dependence on n_i.

We conclude by emphasizing the similarity and the difference between BLG and SLG transport from the perspective of our transport-theory considerations. We find that both manifest a nonuniversal sample-dependent minimum conductivity at the CNP arising from the electron-hole puddle formation due to the presence of long-range Coulomb disorder. We find that BLG manifests a fairly strong insulating temperature dependence of $\sigma_{\min}$. We find that at high density both BLG and SLG manifest a linearly increasing conductivity with increasing carrier density, as observed experimentally. However the physical origin for this linear dependence is quite different in the two systems: while in the SLG this linearity arises entirely from Coulomb disorder, in the BLG the short-range disorder scattering contributes to this linearity. The short-range disorder leads to a strong insulating temperature dependence of BLG conductivity since short-range disorder leads to a $\sigma(T)$ increasing with T for all T, whereas Coulomb scattering always leads to a $\sigma(T)$ decreasing (linearly at first) with increasing T for $T \ll T_F$. The importance of short-range disorder in determining the bilayer conductivity at all densities, in contrast to the corresponding SLG case which is dominated by Coulomb scattering, arises from the qualitatively different density of states in BLG (constant) versus in SLG (linear), thus leading to much stronger effective short-range scattering in BLG compared with SLG even for the same bare scattering strength. We predict in general a nonuniversal density and temperature dependence of BLG conductivity since long- and short-range disorders, with distinct density and temperature dependence both contribute to BLG transport equivalently at all carrier densities.

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