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Universal conductance fluctuations in Dirac materials in the presence of long-range disorder

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We study quantum transport in Dirac materials with a single fermionic Dirac cone (strong topological insulators and graphene in the absence of intervalley coupling) in the presence of non-Gaussian long-range disorder. We show, by directly calculating numerically the conductance fluctuations, that in the limit of very large system size and disorder strength, quantum transport becomes universal. However, a systematic deviation away from universality is obtained for realistic system parameters. By comparing our results to existing experimental data on $1/f$ noise, we suggest that many of the graphene samples studied to date are in a non-universal crossover regime of conductance fluctuations.

With the successful isolation of graphene [1], and the discovery of topological insulators (TI), the study of *Dirac materials* has come to the fore. In a Dirac material, the conduction and valence bands touch at an isolated set of points, called Dirac points (DP) (or *valleys*). The energy spectrum close to the DPs is linear and the low energy properties of these materials are well described by a set of massless 2D Dirac fermions. Graphene is intrinsically a 2D material [2], while in the case of a 3D topological insulator the Dirac fermions are realized as surface states whose presence is demanded by the non trivial topology of the bulk energy bands [3]. In this work, we report an exact numerical theoretical study of quantum conductance fluctuations (CF) in the presence of non-Gaussian long-range disorder in 2D Dirac materials, which should apply directly to both graphene (in the absence of intervalley scattering) and TI surface states. Specifically by (non-Gaussian) long-range disorder we refer to disorder whose spatial correlation function decays algebraically. In *conventional* parabolic band 2D electron liquids, taking into account screening, the disorder potential is short-range even when due to charge impurities. In Dirac materials, in contrast, due to the massless nature of the fermionic excitations, the disorder potential due to charge impurities retains its long-range nature even when screening is taken into account; in particular the spatial correlation function decays as $1/r^3$ at large distances. As a consequence our work is the first to address the very fundamental and broad question of how the long-range nature of the disorder affects the quantum transport properties of 2D electron systems.

In graphene the dominant source of disorder is believed to be from remote charge impurities [2] (though other scattering mechanisms might also be of relevance in certain cases [4]). This type of disorder does not couple the two valleys of graphene and to a good approximation graphene can be described by a single Dirac fermion. At

the same time, a *strong* TI is characterized by an odd number of Dirac cones in the surface spectrum (as opposed to a *weak* TI which has an even number). The dominant physics is captured by the case of a single Dirac fermion which is experimentally realized in *e. g.* Bi_2Se_3 . In both cases the Hamiltonian is invariant under a time reversal symmetry \mathcal{T} with $\mathcal{T}^2 = -1$, placing these systems in the symplectic (AII) symmetry class [5]. Below we focus on the single Dirac fermion case.

In the clean case, the density of states goes to zero and transport is by quantum tunneling of evanescent modes rather than diffusion of propagating modes. This regime is referred to as *pseudo-diffusive* [6]. Disorder drives the system away from the pseudo-diffusive regime and into a symplectic metal phase characterized by weak anti-localization [7] (enhanced conductivity due to destructive interference of time reversal symmetric paths [8]).

These conclusions were reached by studying the effects of short range disorder. However in a Dirac material the disorder potential created by charge impurities retains its long range character even after screening has been taken into account [9]. This leads to strong carrier density inhomogeneities and, close to the DP it induces *puddles* of electrons and holes. In this regime, conventional analytical methods fail and one needs to rely on numerical simulations. This puddle formation due to random charged impurities in the environment has been experimentally observed both in graphene [10] and TIs [11].

In this paper we study the problem of quantum transport in the presence of long range disorder both in the puddle regime and away from the DP at large carrier density, n . We study both quantum corrections to the average conductivity (σ) [weak anti-localization (WAL)] and the CF arising from changes in interference patterns as external parameters are varied. In conventional semiconductors and metals the amplitude of these fluctuations is a universal number giving rise to *universal conduc-*

tance fluctuations (UCF). In terms of the scaling function $\beta(\sigma) = d \ln \sigma / d \ln L$, where L is the sample length, the WAL is the first order term in the expansion in an expansion in $1/\sigma$. It happens that the second and third order terms are identically zero in the symplectic class [12] and therefore the WAL can be obtained already for rather small values of σ . In contrast, higher order terms in the UCF are expected to be nonzero making the numerical calculation of UCF more sensitive to finite size effects. Moreover, in general, the calculation of CF requires a much larger number of disorder realizations than the calculation of σ . These facts make the numerical calculation of CF in the symplectic class much more challenging than the calculation of σ and WAL corrections. Earlier numerical studies [13] of UCF in graphene using tight binding models with short range disorder found results consistent with the UCF theory [14], however, even for short-range disorder, no systematic study of density dependence or deviations from universality was attempted.

We demonstrate that just as in the case of short range Gaussian disorder, long range disorder drives the system into the symplectic metal phase. However, the crossover regime before the universal quantum transport sets in is considerably larger than in the case of short range disorder. This gives rise to CF with an amplitude which is smaller than the UCF close to the DP but considerably larger at high n which, as we argue, can lead to an intriguing non-monotonic behavior of the $1/f$ noise, which may have already been observed in graphene. We emphasize that our study is performed at zero temperature, in the absence of inelastic scattering, conditions in which the phase coherence length l_{ph} is infinite. Our analysis is valid as long as $l_{ph} > L$. The main goal of our work is to study the effect of the long-range nature of the disorder on the universal properties of quantum transport, for this reason we must have $l_{ph} > L$ otherwise sample-dependent effects due to finite l_{ph} would mask the sought after effects. Moreover, any quantum transport measurement strives to be in this regime that appears also to be the relevant one for current experiments on mesoscopic samples of graphene.

To obtain the conductance G of a single Dirac fermion we solve, using the transfer matrix method described in Ref. [7], the scattering problem defined by the Hamiltonian: $H = v_F \mathbf{p} \cdot \boldsymbol{\sigma} + V_D(\mathbf{r}) - \mu$. Here v_F is the Fermi velocity, $\boldsymbol{\sigma}$ the vector formed by the Pauli matrices (σ_x, σ_y) (in spin space for TIs and in sublattice space for graphene), μ the chemical potential which controls n , and V_D is the disorder potential. We take a sample of length L and width W with periodic boundary conditions in the transverse direction. The solution of the scattering problem returns the transmission amplitudes t that in turn give us the two-terminal conductance $G = R^{-1} = (g_s g_v e^2 / h) \text{Tr}(t^\dagger t)$, R being the resistance and g_s and g_v the spin and valley degeneracies respectively ($g_s g_v = 4$ for graphene and $g_s g_v = 1$

for an STI). In the remainder for concreteness we set $g_s g_v = 4$. The conductivity is obtained via the relation $\sigma = (W d R / d L)^{-1}$ which minimizes the contribution of contact resistance [15]. The CF are in turn obtained as the variance $\langle (\delta G)^2 \rangle = \langle G^2 \rangle - \langle G \rangle^2$, where the angle brackets denote the average over disorder realizations.

The scattering potential V_D is induced by the remote impurity charges. In the absence of screening, in momentum space, $V_D(\mathbf{q}) = (e^2 / \epsilon) A(\mathbf{q}) e^{-q d} / q$, where ϵ is the background dielectric constant, d the average distance of the impurities from the graphene layer, and $A(\mathbf{q})$ are random numbers with Gaussian distribution such that $\langle A \rangle = 0$ and $\langle A^2 \rangle = n_{\text{imp}}$, with n_{imp} the impurity density. The bare disorder is renormalized by the interactions replacing the dielectric constant ϵ by a dielectric function $\epsilon \rightarrow \epsilon(\mathbf{q})$. To calculate $\epsilon(\mathbf{q})$ in the presence of charge impurities we use the Thomas Fermi Dirac Theory (TFD) in which both Hartree and exchange-correlation terms are taken into account [16, 17]. The TFD approach is valid when the inequality $|\nabla n| / |n| < k_F$ is satisfied. Close to the DP, due to the disorder, the root mean square of n ($n^{(\text{rms})}$) is much larger than its average. In this situation $n^{(\text{rms})}$ should be used instead of n in the inequality above to verify the validity of the TFD theory [16, 18]. Because $n^{(\text{rms})} \approx n_{\text{imp}}$ [16, 19] the TFD theory is valid as long as n_{imp} is not too small ($\gtrsim 10^{11} \text{cm}^{-2}$) [18, 20]. The TFD gives results for the carrier density profile $n(\mathbf{r})$ and $\epsilon(\mathbf{q})$ that compare well with both density functional theory (DFT) results [21] and experiments [10] and is the only method available, for large samples and ensembles, that takes into account nonlinear screening effects that dominate close to the DP.

For purposes of comparison it is useful to consider different models of screening. In particular one can turn off exchange-correlation terms in the TFD. We denote the corresponding dielectric function by ϵ_{NXC} , the full TFD dielectric function being ϵ_{TFD} . The cases of doping dependent but uniform screening $\epsilon^{-1} \rightarrow \epsilon_{dds}^{-1} = q / (q + 4r_s \mu)$, and constant screening $\epsilon^{-1} \rightarrow \epsilon_{cs}^{-1} = q / (q + q_s)$ will also be considered. Finally, we also compare with the case of Gaussian correlated disorder defined by $\langle V_D(\mathbf{r}) V_D(\mathbf{r}') \rangle = K_0 / (2\pi \xi^2) \exp(-|\mathbf{r} - \mathbf{r}'|^2 / 2\xi^2)$. K_0 is a dimensionless measure of the disorder strength and ξ the correlation length. This is the type of disorder correlation considered in most prior numerics, and in analytical considerations (where the limit $\xi \rightarrow 0$ is routinely taken).

The analytical theory of UCF requires diffusion, i.e. $L \gg \ell$, where ℓ is the mean free path. In this limit one can perform a controlled diagrammatic calculation of transport properties. Adapting the results of the short-range calculation in [14] to our geometry, this approach predicts a universal (independent of microscopic param-

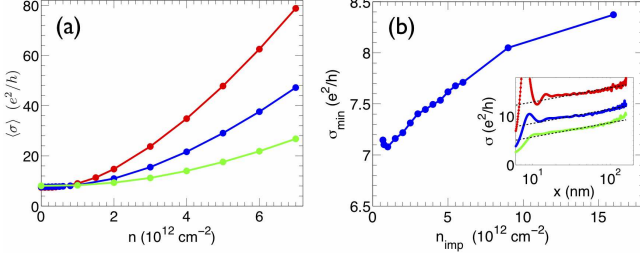


FIG. 1. (Color online). (a) $\langle\sigma\rangle$ as a function of n for $n_{\text{imp}} = (3, 5, 9) \times 10^{12} \text{ cm}^{-2}$ from top to bottom. (b) $\langle\sigma\rangle$ at the DP as a function of n_{imp} for the case of Coulomb disorder. The inset shows $\langle\sigma\rangle$ as a function of sample length L for $W = 160 \text{ nm}$, and $n = (3, 2, 1) \times 10^{12} \text{ cm}^{-2}$ from top to bottom. The dashed lines show $d\sigma/d\ln L = 4e^2/\pi h$.

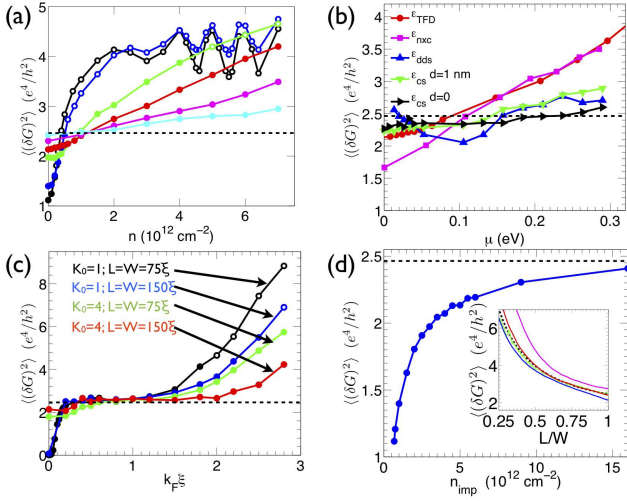


FIG. 2. (Color online). (a) $\langle(\delta G)^2\rangle$ as function of n for the case of long-range disorder ($L = 160 \text{ nm}$) and different values of n_{imp} ; from top to bottom (for $n = 2 \times 10^{12} \text{ cm}^{-2}$): $n_{\text{imp}} = (0.682, 1, 3, 5, 9, 16) \times 10^{12} \text{ cm}^{-2}$. (b) $\langle(\delta G)^2\rangle$ as a function of μ for different types of disorder potential (see text). (c) $\langle(\delta G)^2\rangle$ as a function of $k_F\xi$ for Gaussian disorder. (d) $\langle(\delta G)^2\rangle$ at the DP as a function of n_{imp} for the case of long-range disorder ($L = 160 \text{ nm}$). In the inset $\langle(\delta G)^2\rangle$ as a function of L/W ; the top line shows the results for $n_{\text{imp}} = 5 \times 10^{12} \text{ cm}^{-2}$ and $n = 3 \times 10^{12} \text{ cm}^{-2}$; the solid line below, and the bottom one, show the results for the same n_{imp} and $n = 10^{12} \text{ cm}^{-2}$ and $n = 0$ respectively. Between these two lines there is the line showing the results for the case of Gaussian disorder with $K_0 = 1$ and $k_F\xi = 0.8$.

eters, such as n_{imp} , K_0 and ξ) value of the CF given by

$$\langle(\delta G)^2\rangle_{\text{ucf}} = \left(\frac{e^2}{\pi^2 h}\right)^2 \sum_{n_x=1}^{\infty} \sum_{n_y=-\infty}^{\infty} \frac{12g_sg_v}{\left[n_x^2 + 4\left(\frac{L}{W}\right)^2 n_y^2\right]^2}. \quad (1)$$

Fig. 1(a) shows the dependence of $\langle\sigma\rangle$ on the doping n for three different values of n_{imp} . $\langle\sigma\rangle$ approaches linear

dependence on n at large densities in qualitative agreement with previous theoretical results [18, 22] and experiments [23]. At the DP, the conductivity (σ_{min}) is enhanced by disorder, see Fig. 1(b), in contrast to what is obtained in Boltzmann type of theories extended to the DP, but in agreement with simulations with short range disorder. For large system sizes and disorder strengths σ increases logarithmically with system size, as shown in the inset of Fig. 1(b), consistent with weak anti-localization which predicts $\sigma \sim (g_sg_v/\pi) \ln L$ [24].

Fig. 2(a) shows $\langle(\delta G)^2\rangle$ as a function of n for several values of n_{imp} . The dashed lines in Fig. 2 show the universal value of Eq. (1). We observe that close to the DP the CF tend to be smaller than the UCF value, while at large n they are larger. As n_{imp} is increased, the CF approach the universal value with the set of curves crossing roughly at the UCF value. Similar trends are observed as a function of system size. This suggests that in the thermodynamic limit the CF in the presence of long range disorder, approach the universal value *independent* of n . In this limit the diffusive symplectic metal is an accurate description of the system. In contrast, percolation predicts CF larger than UCF at the DP [25].

To understand better the deviation from universality and to quantify the behavior observed in Fig. 2 we estimate ℓ using the Boltzmann theory, which gives $\ell = f(r_s, k_F d) \sqrt{n}/n_{\text{imp}}$, [9], where $r_s = e^2/(\epsilon\hbar v_F)$ and f is a function that for $d \lesssim 1 \text{ nm}$ depends very weakly on $k_F d$ [22, 26]. For $d = 1 \text{ nm}$ and $r_s = 0.8$, $f \approx 5.66$ almost independent of k_F . In Fig. 2 we represent with open symbols those data points for which $\ell > 0.25L$, revealing that the observed oscillations at large n and small n_{imp} are ballistic effects. It also suggests that the departure of the CF from the UCF value at high n is due to the fact that we are in the ballistic to diffusive crossover regime. Similarly, close to the DP, the deviations are attributed to a pseudo-diffusive to diffusive crossover (the estimates of ℓ are not as reliable in this regime).

To better understand the role played by the disorder-induced density inhomogeneities we plot in Fig. 2(b) the CF for the different variants of screening discussed above. We observe that neglecting exchange-correlation terms in the TFD increases the deviation of the CF from the universal value close to the DP. This is due to the fact that in the absence of exchange-correlation the amplitude of the density fluctuations are increased [21]. In contrast, assuming uniform screening, either doping dependent or constant, gives results that are closer to the UCF value. The results of Fig. 2(b) clearly show that the presence of strong carrier density inhomogeneities increases the range of n and n_{imp} for which the transport is in the crossover regime for which the CF differ from the universal value.

In Fig. 2(c) we show the CF for the gaussian correlated potential as a function of $k_F\xi = (4\pi n/g_sg_v)^{1/2}$. In this case from the Boltzmann theory we have $\ell =$

$2\sqrt{2}\pi\xi^3k_F^2/K_0$. As in the case of charge impurities we find that in the pseudo-diffusive regime $\langle(\delta G)^2\rangle$ is smaller than the UCF value, and larger in the ballistic high density regime, but approaches the UCF value as the impurity strength K_0 or system size L are increased. In contrast to the long range case, there is a large range of intermediate values of n where the CF quickly goes to the UCF value. Thus, the crossover regime is strongly suppressed for short-range disorder compared with long-range disorder. In the presence of spatial correlations among charge impurities the long-range nature of the disorder is suppressed compared to the case of uncorrelated impurities [27] and so we predict that the crossover regime will also be reduced.

The trend that emerges from Fig. 2(a) is that as n_{imp} increases the CF approach the universal value. This is further demonstrated in Fig. 2(d) which shows the value of the CF at the DP as a function of n_{imp} for the case of charge impurities. We see that for very large n_{imp} , for which $\ell/L \ll 1$, the CF saturate to the universal value (dashed line). In the inset to Fig. 2(d) we compare the aspect ratio dependence of the CF to the analytical expression (1). Both in the case of long range and Gaussian disorder the curves agree well within the universal regime. In the crossover regime the CF follow the same trend but with an amplitude that differs from the UCF prediction.

Taken together these results suggest that even in the presence of long-range disorder, the system is eventually (large enough L and/or disorder strength) driven into the universal symplectic metal phase and that, however, the crossover regime in which neither ballistic or universal diffusive physics is applicable is very large in the presence of long-range Coulomb disorder and puddles.

To connect these results with experiments we consider the relevance of the CF results to the $1/f$ noise. In 2D (and 1D) the displacement of a single defect can cause a change in G of the order of e^2/h [28]. One of the probable sources of resistance fluctuations is thermally activated motion of defects. Assuming that the defects move on a time scale $\tau \gg \tau_{\text{inelastic}}$ and that the hopping distance is uncorrelated with τ , for the spectrum of the resistance fluctuations $S_R(\omega) = \int dt \langle \delta R(t) \delta R(0) \rangle e^{i\omega t}$ we have [28]

$$S_R(\omega) = R^2 \left[\frac{\langle(\delta G)^2\rangle}{\langle G \rangle^2} \right] \int \frac{2\tau}{\omega^2\tau^2 + 1} P(\tau) d\tau \quad (2)$$

where $P(\tau)$ is the probability distribution of the time that it takes a defect to move. If the motion of defects is thermally activated then $P(\tau)$ is quite broad and $S_R(\omega)$ will be approximately $1/f$. We can then calculate the strength of the $1/f$ noise by calculating the coefficient $\langle(\delta G)^2\rangle/\langle G \rangle^2$, or equivalently $\langle(\delta G)^2\rangle/\langle \sigma \rangle^2$.

Fig. 3 shows $\langle(\delta G)^2\rangle/\langle \sigma \rangle^2$ as a function of n for both charge disorder and Gaussian disorder. In both cases we see that at low disorder strengths $\langle(\delta G)^2\rangle/\langle \sigma \rangle^2$ depends non-monotonically on n . The reason is that in

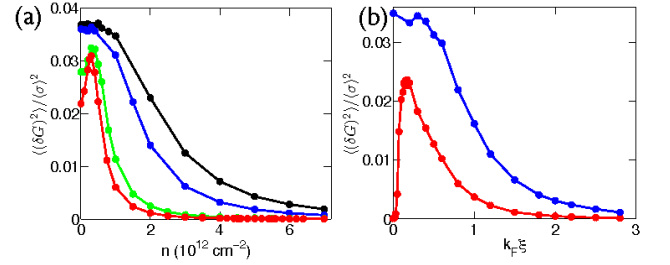


FIG. 3. (Color online). (a) $\langle(\delta G)^2\rangle/G^2$ as function of n for the case of long-range disorder ($L = W = 160 \text{ nm}$) and different values of n_{imp} ; from top to bottom (for $n = 2 \times 10^{12} \text{ cm}^{-2}$): $n_{\text{imp}} = (5, 3, 1, 0.682) \times 10^{12} \text{ cm}^{-2}$. (b) $\langle(\delta G)^2\rangle/G^2$ as a function of $k_F \xi$ for the case of Gaussian disorder for $K_0 = 4$, top, and $K_0 = 1$, bottom. $L = W = 75\xi$.

the pseudo-diffusive regime $\langle(\delta G)^2\rangle$ grows rapidly with n while G grows very slowly, whereas at larger values of n the transport is diffusive and $\langle(\delta G)^2\rangle$ is almost constant while G grows rapidly with n . In contrast, in the symplectic metal regime the ratio $\langle(\delta G)^2\rangle/\langle \sigma \rangle^2$ decreases monotonically with n . We conclude that the non-monotonic dependence of the $1/f$ noise is a generic property of the crossover regime between pseudo-diffusive and diffusive regimes. The $1/f$ noise of graphene has been measured experimentally [29] and its dependence on n has been shown to qualitatively follow the non-monotonic behavior shown in Fig. 3. This suggests that the samples in these experiments are not fully in the diffusive regime but rather in a non-universal crossover regime.

In conclusion, we have calculated the amplitude of the conductance fluctuations in Dirac materials with a single Dirac cone and in the presence of disorder with various range and screening properties. Our work is the first to consider the effect of the long-range nature of disorder on the quantum transport properties of 2D electron systems. In the limit that the mean free path is much smaller than the system size, the CF approach the universal value predicted by diagrammatic calculations. Before reaching the universal value the CF are systematically smaller than the universal value close to the DP but larger away from it. In particular, for system parameters realistic to graphene, the CF seems to deviate from the universal value leading to a non-monotonic dependence of $1/f$ noise, as recently observed in experiments [29].

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