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Effects of long-range correlated disorder on Dirac fermions in graphene

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We study two-dimensional transport of quasirelativistic electronic excitations in graphene in the presence of Coulomb impurities and topological structural defects described by static long-range-correlated random scalar and vector potentials, respectively. Our results for the transport and cyclotron rates as well as the decay rate of the Friedel oscillations provide the means of identifying the dominant scattering mechanism in graphene. We also discuss the properties of zero-energy states and pertinent localization scenarios.

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In recent years, the theory of electron localization in two dimensions (2D) has been extended to the situation where, instead of (or in addition to) a random potential (RP), there exists a random magnetic field (RMF). This type of problem emerges in the context of compressible quantum Hall states,[1] finite-temperature dynamics of spin liquid states in Mott insulators,[2] and the vortex line liquid phase in high-T_c cuprates,[3] to name a few.

The recently discovered graphene provides yet another application of this disorder model. Although a number of different (anti)localization-related phenomena in graphene have already been discussed,[4,5] these studies were limited to the case of short-range (albeit, possibly, arbitrarily strong) disorder. Despite its technical convenience, however, the latter assumption is not applicable to graphene, as suggested by such experimental evidence as the linear electron density dependence of the conductivity,[6] which appears to be inconsistent with the predictions based on the model of short-range disorder.[7]

The recent work of Ref. 7 invoked the effect of long-range Coulomb impurities residing in the SiO_2 substrate in order to explain the data of Ref. 6. Independently, it has also been pointed out that besides the Coulomb ("scalar") RP, graphene possesses a "vector" (RMF) disorder representing topological defects, such as disclinations (isolated pentagon and heptagon rings), dislocations (pairs of adjacent pentagons and heptagons), and Stone-Wales defects (double pairs).[8] The presence of structural defects in free-standing graphene is inevitable due to the intrinsic thermodynamic instability of 2D crystals.

In previous work, the RMF in graphene was repeatedly treated as being short range in terms of the vector potential (rather than the magnetic field itself), which simplification facilitates the use of the powerful machinery of the renormalization group[8] and 2D conformal field theory.[9]

By contrast, in the present Rapid Communication we study the effects of a genuine long-range-correlated RP and RMF on electron transport in graphene and contrast the results with those pertaining to the conventional 2D electron gas (2DEG) with parabolic electron dispersion. The main goal of our analysis is to develop the means of ascertaining the dominant mechanism of elastic scattering in graphene.

The low-energy Dirac-like quasiparticle excitations residing near two conical points (K and K') in the hexagonal Brillouin zone of graphene are described in terms of the (retarded) Green function

$$\hat{G}^R(\omega,\mathbf{p}) = \frac{(\epsilon+\Sigma^R)\hat{\gamma}_0 + v\hat{\gamma}\mathbf{p}}{(\epsilon+\Sigma^R)^2 - v^2\mathbf{p}^2}, \quad (1)$$

where v is the Fermi velocity and the 4×4 $\hat{\gamma}$ matrices $\hat{\gamma}_\mu = (i\mathbf{1}\otimes\sigma_3, \mathbf{1}\otimes\sigma_2, -\sigma_3\otimes\sigma_1)$ act in the space of the Dirac bispinors $\psi=(\psi_K(A),\psi_K(B),\psi_{K'}(A),\psi_{K'}(B))$ composed of the values of the electron wave function on the A and B sublattices of the bipartite lattice of graphene.

These Dirac fermions are subject to random scalar (s) and vector (v) fields whose spatial correlations are controlled by the Gaussian averages

$$\langle a_\mu(\mathbf{q})a_\nu(-\mathbf{q})\rangle = \delta_{\mu0}\delta_{\nu0}w_s(\mathbf{q}) + \delta_{\mu i}\delta_{\nu j}w_v(\mathbf{q})\left(\delta_{ij} - \frac{q_iq_j}{\mathbf{q}^2}\right). \quad (2)$$

The variances $w_{s,v}(\mathbf{q})=4\pi^2\Gamma_{s,v}/\mathbf{q}^2$ are proportional to the areal densities of the Coulomb impurities ($\Gamma_s=g^2n_i$ where $g=e^2/\varepsilon_0 v$ is the Coulomb interaction parameter) and topological defects ($\Gamma_v\sim n_d$), respectively.

Strictly speaking, in the case of graphene the vector field $\vec{\mathbf{a}}$ becomes a 4×4 matrix,[10] thus endowing Eq. (2) with the structure of a 16×16 matrix. It appears, however, that this technical complication does not affect any of the qualitative results presented below and, therefore, we will use Eq. (2) as is from now on.

A preliminary insight into the problem can be gained by attempting to compute the fermion self-energy in the framework of the customary self-consistent Born approximation (SCBA)

$$\hat{\Sigma}^R_\alpha(\epsilon,\mathbf{p}) = \int\frac{d\mathbf{q}}{(2\pi)^2}\frac{w_\alpha(\mathbf{q})}{\hat{G}^R(\epsilon,\mathbf{p}+\mathbf{q})^{-1} + \hat{\Sigma}^R_\alpha(\epsilon,\mathbf{p}+\mathbf{q})}. \quad (3)$$

In the case of the RP, the singular behavior of $w_s(\mathbf{q})$ at $q\to0$ gets replaced by $w_s(\mathbf{q})=\Gamma_s/(q+\kappa)^2$ due to the Debye screening. The corresponding Debye momentum $\kappa=4gp_F$ proportional to the Fermi surface radius $p_F=(\pi n_e)^{1/2}$, where n_e is the density of excess electrons with respect to half filling, renders the corresponding quasiparticle width finite:

$$\gamma_s = \mathrm{Im}\,\mathrm{Tr}\,\hat{\gamma}_0\hat{\Sigma}^R_s(\epsilon,\epsilon/v) \sim \frac{v^2\Gamma_s}{\epsilon}\min\left[\frac{1}{g},\frac{1}{g^2}\right]. \quad (4)$$

By contrast, a calculation of the self-energy associated with the RMF is impeded by the lack of screening for the random vector potential, which results in an infrared divergence:

$$\gamma_v = \mathrm{Im}\,\mathrm{Tr}\,\hat{\gamma}_0 \hat{\Sigma}_v^R(\epsilon, \epsilon/v) \sim v\Gamma_v^{1/2}\sqrt{\ln L} \tag{5}$$

where L is the size of the system.

This intrinsic divergence cannot be avoided even if one proceeds beyond the SCBA, for it stems from the non-gauge-invariant nature of the fermion Green function $\hat{G}^R(t,\mathbf{r})$ for $\mathbf{r}\neq\mathbf{0}$. Taken at its face value, the divergent self-energy (5) is indicative of a strongly non-Lorentzian form of the RMF-averaged Green function.[11]

It is worth mentioning that, unlike in the previously discussed examples of the RMF problem involving some auxiliary fermions that are different from physical electrons,[1–3] in the present case there is no physical ground for replacing the original Green function (1) with a gauge-invariant amplitude such as, e.g., $\hat{\mathcal{G}}^R(t,\mathbf{r}) = <\psi(t,\mathbf{r})\exp(-i\int_C \mathbf{a}(\mathbf{r}')d\mathbf{r}') \times \psi^\dagger(0,0)>$.

Nonetheless, Eq. (3) can be used to evaluate the Drude transport rates in both RP and RMF cases. Inserting the factor $1-\cos\theta$ related to the transferred momentum $q = 2p\sin\theta/2$ into the integrand in Eq. (3) and putting $\epsilon=\epsilon_F = vp_F$, one obtains the first-order Born estimates

$$\gamma_\alpha^{tr} = \int \frac{d\mathbf{q}}{(2\pi)^2}\delta(\epsilon_F - v|\mathbf{p}+\mathbf{q}|)w_\alpha(\mathbf{q})(1-\cos\theta), \tag{6}$$

which both turn out to be finite,

$$\gamma_s^{tr} \sim \frac{v^2\Gamma_s}{\epsilon_F}\min\left[1,\frac{1}{g^2}\right], \quad \gamma_v^{tr} \sim \frac{v^2\Gamma_v}{\epsilon_F}, \tag{7}$$

and inversely proportional to $n_e^{1/2}$, thereby giving rise to the Drude conductivity $\sigma \propto n_e$, in agreement with experiment[6] (note that the experimentally relevant value of the Coulomb coupling is $g\sim 1$), and in contrast to the situation in the conventional 2DEG where the transport rate $\gamma_\alpha^{tr} \sim \Gamma_\alpha/m$ depends on the band mass m, thus yielding $\sigma \propto n_e^{1/2}$.

To make further progress, we employ a path-integral representation of the Dirac fermion Green function which was devised in Ref. 12:

$$G^R(\epsilon,\mathbf{r}|a_\mu(\mathbf{r})) = \int_0^\infty dt \int_{\mathbf{r}(0)=\mathbf{0}}^{\mathbf{r}(t)=\mathbf{r}} D\mathbf{r}\,D\mathbf{p} \times \exp\left(i\hat{S}_0(t) + i\int_0^t d\tau [a_0(\mathbf{r})] - \frac{d\mathbf{r}}{d\tau}[\mathbf{A}+\mathbf{a}(\mathbf{r})]\right) \tag{8}$$

where A_μ represents the external field (if any) and the free Dirac action reads

$$\hat{S}_0(t) = \int_0^t d\tau\left[\epsilon\hat{\gamma}_0 + \mathbf{p}\left(\frac{d\mathbf{r}}{d\tau} - \hat{\gamma}\right)\right]. \tag{9}$$

In Eq. (8), the usual ordering of $\hat{\gamma}$ matrices with respect to the proper time τ must be performed according to the order of their appearance in the series expansion of the exponent. In contrast to various approximate (e.g., Bloch-Nordsieck) representations, the integration over the momentum $\mathbf{p}(\tau)$ conjugate to the spatial coordinate $\mathbf{r}(\tau)$ allows one to account for the spinor structure of the fermion propagator (1) exactly.

Averaging over the disorder variables introduces a product of the "Debye-Waller" attenuation factors into the integrand in Eq. (8) [here $u_\mu = (1, d\mathbf{r}/d\tau)$]

$$W_\alpha[\mathbf{r}(\tau)] = \exp\left(-\frac{1}{2}\int \frac{d\mathbf{q}}{(2\pi)^2}\int_0^t d\tau \int_0^t d\tau' \times \mathbf{u}_\mu(\tau)\mathbf{u}_\nu(\tau')\langle a_\mu(\mathbf{q})a_\nu(-\mathbf{q})\rangle e^{i\mathbf{q}[\mathbf{r}(\tau)-\mathbf{r}(\tau')]}\right). \tag{10}$$

Despite its generally non-gauge-invariant nature, the amplitude (8) does appear to be gauge invariant for closed trajectories ($\mathbf{r}=0$), thus allowing one to analyze such magnetotransport effects as de Haas–van Alfven (dHvA) [Shubnikov–de Hass (SdH)] oscillations of the density of states (hence magnetization, etc.) and conductivity in a weak uniform external magnetic field $B \ll \Gamma_{s,v}$.

Evaluating Eq. (8) on the semiclassical trajectories which dominate the path integral and correspond to multiple repetitions of the Larmor orbit of radius $R_c = \epsilon/vB$, one obtains a field-dependent density of states

$$\nu(\epsilon|B) = \nu(\epsilon|0)\sum_{n=-\infty}^{\infty} e^{2\pi i n A(\epsilon) - n^2\delta S_1(\epsilon)}, \tag{11}$$

where $A(\epsilon) = \pi\epsilon^2/B$ is the area of the Larmor orbit and the attenuation factor contributes as

$$\delta S_1(\epsilon) = -\sum_{\alpha=s,v}\ln W_\alpha = \pi\left(\frac{\Gamma_s}{B} + \frac{\Gamma_v\epsilon^2}{v^2B^2}\right), \tag{12}$$

which allows one to identify the proper cyclotron rates

$$\gamma_s^{cycl} \sim v\Gamma_s^{1/2}, \quad \gamma_v^{cycl} \sim (\epsilon^2 v^2\Gamma_v)^{1/4}, \tag{13}$$

associated with the linear and quadratic (in powers of $1/B$) Dingle plots, respectively. These results should be contrasted with their "nonrelativistic" counterparts $[\gamma_s^{cycl} \sim \Gamma_s/m, \gamma_v^{cycl} \sim (\epsilon\Gamma_v/m)^{1/2}]$.

The path integral technique is also well suited for analyzing various gauge-invariant two-particle amplitudes. For one, the ballistic Drude conductivity manifesting the transport rates (7) can be found by computing the average $<\hat{G}^R(\epsilon,\mathbf{r})\hat{G}^A(\epsilon,-\mathbf{r})>$ in the semiclassical approximation. Expanding the corresponding path integral about a proper semiclassical trajectory (see below), one can systematically study ballistic corrections to the Drude conductivity. Due to the long-range nature of the RMF disorder, these corrections do not appear to be logarithmic and, therefore, are not readily amenable to a simple resummation via renormalization group (compare with the case of short-range disorder[5]).

Another example of a relevant two-particle amplitude is given by the correlation function of the electron wave functions' amplitudes related to the average,[13]

$$\langle \hat{G}^R(\epsilon,\mathbf{r})\hat{G}^R(\epsilon,-\mathbf{r})\rangle = \prod_{i=1,2}\int_0^\infty dt_i \int_{\mathbf{r}_i(0)=0}^{\mathbf{r}_i(t_i)=\pm\mathbf{r}} D\mathbf{r}_i D\mathbf{p}_i \times e^{i\hat{S}_0(t_1)}e^{i\hat{S}_0(t_2)}\prod_{\alpha=s,v}\prod_{i,j=1,2} W_\alpha[\mathbf{r}_i(\tau_1) - \mathbf{r}_j(\tau_2)]. \quad (14)$$

Observe that the product of the W_v factors yields an exponent of the Amperian area of a contour formed by the trajectories $\mathbf{r}_1(\tau)$ and $-\mathbf{r}_2(\tau)$.

In the ballistic regime, Eq. (14) receives its main contribution from the pairs of trajectories with single-valued projections onto the semiclassical straight-path trajectory $\mathbf{r}^{(0)}\times(\tau)=\mathbf{r}\tau/t$.[2,13] Therefore, one can separate out the coordinate variables into the center-of-mass and relative ones ($\mathbf{r}^{\pm}=\mathbf{r}_1\pm\mathbf{r}_2$, $\mathbf{p}^{\pm}=\mathbf{p}_1\pm\mathbf{p}_2$), expand up to the second order in $\mathbf{r}^-$ and $\mathbf{p}^-$, and integrate over all the variables except for the transverse deviation from the straight path $x_\perp^-(\tau)$, thus arriving at the disorder-induced correction to the free Dirac action

$$\delta S_2(t) = \int_0^t d\tau\{\Gamma_s\epsilon[x_\perp^-(\tau)]^2 + \Gamma_v v|x_\perp^-(\tau)|\}. \quad (15)$$

Comparing typical values of the free fermion action and the correction (15), we find that the condition $S_0 \gg \delta S$, under which the path integral (14) would be dominated by the trajectories close to $\mathbf{r}^{(0)}(\tau)$, is readily satisfied in the ballistic regime ($\epsilon \gg v\Gamma_\alpha^{1/2}$).

Thus, in the leading approximation, the amplitude (14) is given by the product of the free Dirac propagator $\hat{G}^R(\epsilon,\mathbf{r}) \sim (1+\hat{\gamma}\mathbf{r}/r)(\epsilon/v^3 r)^{1/2}\exp(i\epsilon r/v)$ (for $\epsilon r/v \gg 1$) and a Fourier transfrom (over the variable $\epsilon - p$) of the Green function $g(x,x'|\epsilon,p)|_{x=x'=0}$ of the 1D equation of motion in the direction perpendicular to the classical trajectory,

$$[v^2\partial_x^2 + (\epsilon + iv\Gamma_v|x| + i\epsilon\Gamma_s x^2)^2 - v^2p^2]g(x,x'|\epsilon,p) = \delta(x-x'). \quad (16)$$

The imaginary effective potential appearing in (16) restrains the transverse Dirac fermion's motion, unlike a real potential, which allows for Klein tunneling.

In the pure RP or RMF case, the solution of Eq. (16) can be presented in the form

$$g_s(0,0|\omega) = \frac{1}{(v^6\epsilon^2\Gamma_s)^{1/4}} f_s\left(\frac{\omega}{v\Gamma_s^{1/2}}\right),$$

$$g_v(0,0|\omega) = \frac{1}{(v^5\epsilon\Gamma_v)^{1/3}} f_v\left(\frac{\omega\epsilon^{1/3}}{v^{4/3}\Gamma_v^{2/3}}\right). \quad (17)$$

In the ballistic regime, the scaling functions $f_{s,v}(z)$ approach the parabolic cylinder and Airy functions, respectively.

The real-space asymptotic behavior of the irreducible part of the wavefunction amplitudes' correlator

$$L^4\langle|\psi^2(\mathbf{r})\psi^2(\mathbf{0})|\rangle - 1 = \frac{\langle \mathrm{Im}\,\hat{G}^R(\epsilon,\mathbf{r})\mathrm{Im}\,\hat{G}^R(\epsilon,-\mathbf{r})\rangle}{(\pi\nu(\epsilon))^2} \sim \left(\frac{\gamma_\alpha^{FO}}{\epsilon^2 r}\right)^{1/2}\cos(2\epsilon r)e^{-r\gamma_\alpha^{FO}} \quad (18)$$

allows one to identify the rates controlling the spatial decay of its Friedel-type oscillations,

$$\gamma_s^{FO} \sim v\Gamma_s^{1/2}, \quad \gamma_v^{FO} \sim v^{4/3}\frac{\Gamma_v^{2/3}}{\epsilon^{1/3}}, \quad (19)$$

and contrast them with their nonrelativistic counterparts ($\gamma_s^{FO} \sim \gamma_s^{tr}$ and $\gamma_v^{FO} \sim \Gamma_v^{2/3}\epsilon^{1/3}/m^{2/3}$).

These rates (equivalently, length scales) are also manifested by other types of Friedel oscillations [which, in principle, can be detected in scanning tunneling microscopy (STM) experiments], such as those of the electron density profile induced by an isolated impurity or the Ruderman-Kittel-Kasuya-Yosida interaction between a pair of magnetic ions. That is, at distances $r \sim v/\gamma_\alpha^{FO}$ the previously found behavior $\delta\rho(r) \propto \cos(2\epsilon r)/r^3$[14] changes to

$$\delta\rho(r) \propto \left(\frac{\gamma_\alpha^{FO}}{r^5}\right)^{1/2}\cos(2\epsilon r)e^{-r\gamma_\alpha^{FO}}. \quad (20)$$

Together with the transport (7) and cyclotron (13) rates, the distinct energy (hence, electron density) dependences presented in Eq. (19) in experiment, all the rates would naturally be evaluated at $\epsilon=\epsilon_F$) can be used to discriminate between the RP and RMF mechanisms of elastic scattering in graphene by performing a combination of transport, magnetization, and STM measurements.

In the complementary low-energy limit ($\epsilon \lesssim v\Gamma_\alpha^{1/2}$), the above eikonal-type approach ceases to be applicable. Nonetheless, one can still gain some insight into the localization properties of the system in question by focusing on zero-energy states (if any).

In the (apparently, more challenging) case of a pure RMF, these states can be explicitly constructed in the form

$$\psi_\pm(\mathbf{r}) \propto (\mathbf{1} \pm \hat{\gamma}_0)\begin{pmatrix} e^{\phi(\mathbf{r})} \\ e^{-\phi(\mathbf{r})} \end{pmatrix} \quad (21)$$

for an arbitrary configuration of the random vector potential parametrized as $a_i(\mathbf{r})=\epsilon_{ij}\nabla_j\phi(\mathbf{r})$.

In a finite system, a degree of the wave functions' localization (or a lack thereof) can be inferred from the inverse participation ratios

$$\mathcal{P}_n = \left\langle \frac{\int |\psi(\mathbf{r})|^{2n}d\mathbf{r}}{L^2\left(\int |\psi(\mathbf{r}')|^2 d\mathbf{r}'\right)^n} \right\rangle \sim \Gamma_v^n, \quad (22)$$

where the Gaussian averaging over the disorder field $\phi(\mathbf{r})$ was performed with the weight $P[\phi(\mathbf{r})] \propto \exp[-\int d\mathbf{r}(\nabla^2\phi)^2/2\Gamma_v]$.

Equation (22) is in stark contrast with that in the short-range case where the zero-energy wave functions demonstrate a prelocalized behavior and the participation ratios exhibit a multifractal spectrum of anomalous dimensions $\mathcal{P}_n \propto L^{-an+bn^2}$.[9]

Taken at its face value, Eq. (22) is suggestive of a possible strong localization of the zero-energy states, the apparent localization length being of order $\sim\Gamma_v^{-1/2}$. If this is indeed the case, it would also be conceivable that all the states up to the energy $\sim v\Gamma_v^{1/2}$ might be localized.

A more familiar framework for studying localization, as manifested by the two-particle amplitudes in the diffusive regime ($|\epsilon_1 \pm \epsilon_2| \lesssim \gamma_\alpha^{tr}$), is provided by the nonlinear σ model (NLσM). In the strongly doped case ($\epsilon_F \gg \gamma_\alpha^{tr}$), a derivation of the corresponding (supersymmetric) NLσM would closely follow the solution of the RMF problem for nonrelativistic spinful fermions with a gyromagnetic ratio equal to 2.[15] This model features the same unitary symmetry as that with only an orbital coupling to the long-range RMF,[16] thus implying localization of all the states.

In that regard, the argument of Ref. 17 that RMF scattering suppresses any quantum coherence between pairs of time-reversed trajectories (which can result in either localizing or antilocalizing behavior, depending on the relative strength of the intra- vs intervalley scattering[4]) would only apply in the case of a smoothly varying (non-Gaussian) RMF.

Indeed, as the aforementioned NLσM analysis suggests, in the case of a Gaussian RMF described by Eq. (2) the onset of localization is merely postponed until greater length scales ($e^{\pi\sigma^2}v/\gamma_v^{tr}$ instead of $e^{\pi\sigma}v/\gamma_v^{tr}$, provided that the bare conductivity $\sigma \gg 1$). It should be noted, however, that by modeling the RMF as a random Gaussian variable with the variance (2), one misses out on the possibility of delocalized semiclassical "snake" trajectories, akin to those found in the case of nonrelativistic fermions in a smoothly varying RMF with the correlation length greater than v/ϵ.[18]

In the opposite (undoped, $\epsilon_F \lesssim \gamma_\alpha^{tr}$) limit, a systematic derivation of the NLσM is impeded by the lack of a suitable expansion parameter, for the bare conductivity takes values of order $\sim e^2/h$. This caveat notwithstanding, it was recently argued that the NLσM description can be applied all the way down to $\epsilon_F=0$, where the corresponding unitary NLσM acquires a topological term which, in the absence of intervalley scattering, precludes localization and drives the system into a critical point characterized by a universal conductivity,[19] in general agreement with the experimental observation of a robust $\sigma(\epsilon_F=0) \approx 4e^2/h^6$.

Considering that the analysis of Ref. 19 was (at least, seemingly) carried out in the default case of a Gaussian disorder described by a momentum-independent correlator, it would be interesting to see if this conjecture still holds for the genuine long-range RMF given by Eq. (2), despite the apparent localizing behavior of the zero-energy states exhibited by Eq. (22) (a negative result would obviously disfavor the topological defects as an important scattering mechanism, as far as the possibility of a finite conductivity at $\epsilon_F=0$ is concerned[19]).

In summary, we studied the behavior of two-dimensional Dirac fermions subject to long-range-correlated random scalar and vector potentials which represent the Coulomb impurities and topological structural defects in graphene, respectively. In the ballistic regime of large quasiparticle energies, we obtain different scattering rates manifested by the Drude conductivity as well as dHvA (SdH) and Friedel oscillations. The distinct energy (density) dependencies of such rates provide a possible means of ascertaining the dominant mechanism of elastic scattering in graphene. Also, in the complementary low-energy regime, we find a signature of strong localization due to a long-range RMF and discuss pertinent (de)localization scenarios.

Our results can also be applied to formally related problems involving disordered Dirac fermions, including that of quasiparticle transport in the vortex line liquid phase of cuprates.

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