Electron Localization Properties in Graphene

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We study localization properties of the Dirac-like electronic states in monolayers of graphite. In the framework of a general disorder model, we discuss the conditions under which such standard localization effects as the logarithmic temperature-dependent conductivity correction appear to be strongly suppressed, as compared to the case of a two-dimensional electron gas with parabolic dispersion, in agreement with recent experimental observations.

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After several decades of predominantly application-driven studies, graphene has finally been recognized as a unique example of the system of two-dimensional fermions with linear dispersion and pseudorelativistic kinematical properties. The recent advances in microfabrication of graphitic samples that are only a few carbon layers thick [1] have made it possible to test the early theoretical predictions of the anomalous properties of this system [2].

The most striking experimental observation up-to-date was that of an unusual (half-integer) quantization of the Hall conductivity [1], which is characteristic of the Dirac nature of the quasiparticle excitations in graphene [3]. The other properties manifesting this peculiar single-particle kinematics have been revealed by magnetotransport measurements [1], including the $\sqrt{B}$ dependence of the energies of (nonequidistant) Landau levels and the intrinsic π shift of the phase of the Shubnikov–de Haas oscillations [4].

A further insight into the properties of electron states in realistic (disordered) graphene can be gained from those single-particle phenomena that involve quantum interference between electronic waves scattered off of multiple impurities. Conceivably, these properties can be affected by the Dirac kinematics, too, and therefore they might be expected to differ from their counterparts in the conventional two-dimensional electron gas (2DEG) with parabolic electron dispersion.

For one, contrary to the situation in the conventional 2DEG, the available experimental data do not manifest any pronounced weak-localization effects even at the lowest accessible temperatures where one would expect the graphene samples to be well in the diffusive regime [5]. Motivated by these findings, in the present work we set out to study electron localization (or a lack thereof) in graphene.

The electronic band structure of graphene is characterized by the presence of a pair of inequivalent nodal points at the wave vectors $\vec{K}_{1,2} = (2\pi/9a)(\pm\sqrt{3}, 3)$, where a is the lattice spacing. At these two and the four other points in the Brillouin zone obtainable from $\vec{K}_{1,2}$ with a shift by one of the reciprocal lattice vectors $\vec{Q}_{1,2} = (2\pi/3a)(\sqrt{3}, \pm 1)$, the valence and conduction bands touch upon each other as a pair of opposing cones with the opening angle given by the Fermi velocity v_F.

In the leading approximation, quasiparticle excitations in the vicinity of the nodal points (hereafter referred to as valleys) can be described by the Dirac Hamiltonian [2]

$$\hat{H} = v_F[\hat{1} \otimes \hat{\sigma}_x k_x + \hat{\tau}_z \otimes \hat{\sigma}_y k_y], \tag{1}$$

where $\hat{\sigma}_i$ is the triplet of the Pauli matrices acting in the space of spinors $\Psi = (\Psi_A, \Psi_B)$ composed of the values of the electron wave function on the A and B sublattices of the hexagonal lattice of graphene, whereas the triplet $\hat{\tau}_i$ acts in the valley subspace. In the absence of magnetic field, the Hamiltonian (1) remains a unity matrix in the physical spin subspace.

In the presence of disorder, the quasiparticles experience both intra- and intervalley scattering. Upon averaging over disorder, the most general form of the elastic four-fermion vertex function is represented by the expression

$$\begin{aligned}\hat{W} = {} & g_4\left[\frac{1+\hat{\tau}_z}{2} \otimes \frac{1+\hat{\tau}_z}{2} + \frac{1-\hat{\tau}_z}{2} \otimes \frac{1-\hat{\tau}_z}{2}\right] \\ & + g_2\left[\frac{1+\hat{\tau}_z}{2} \otimes \frac{1-\hat{\tau}_z}{2} + \frac{1-\hat{\tau}_z}{2} \otimes \frac{1+\hat{\tau}_z}{2}\right] \\ & + g_1[\hat{\tau}_+ \otimes \hat{\tau}_- + \hat{\tau}_- \otimes \hat{\tau}_+] \\ & + g_3[\hat{\tau}_+ \otimes \hat{\tau}_+ + \hat{\tau}_- \otimes \hat{\tau}_-],\end{aligned} \tag{2}$$

where we used the customary notations for the processes of forward scattering between fermions from the same (g_4) and different (g_2) valleys, as well as those of "backward" scattering (g_1) with the momentum transfer close to $\vec{K}_1 - \vec{K}_2$. Besides, we have included the possibility of "umklapp" scattering (g_3) where the total momentum of two fermions changes by $2(\vec{K}_1 - \vec{K}_2) = \vec{K}_2 - \vec{K}_1 + \vec{Q}$. A justification for this (not immediately obvious, considering that the total momentum changes by only a fraction of the reciprocal lattice vector) extension of the disorder model will be discussed later.

In the framework of the self-consistent Born approximation (SCBA), the effect of disorder on the quasiparticle

spectrum is described by the self-energy obeying the equation

$$\hat{\Sigma}^R(\omega,\vec{k}) = \int \frac{d\vec{q}}{(2\pi)^2}\,\mathrm{Tr}\hat{W}\hat{G}^R(\omega,\vec{k}+\vec{q}), \tag{3}$$

where the retarded Green function is given by the expression

$$\hat{G}^R(\omega,\vec{k}) = \frac{(\omega+\mu+\Sigma^R)\hat{1}\otimes\hat{1} + v_F(\hat{1}\otimes\hat{\sigma}_x k_x + \hat{\tau}_z\otimes\hat{\sigma}_y k_y)}{(\omega+\mu+\Sigma^R)^2 - v_F^2 k^2} \tag{4}$$

which includes a chemical potential $\mu > 0$, thus allowing one to account for variable electron density.

Notably, the solution to Eq. (3) turns out to be diagonal in the valley and sublattice subspaces, and its value $\hat{\Sigma}^R(0,0) = i\gamma\hat{1}\otimes\hat{1}$ at $\omega = \vec{k} = 0$ determines the inverse elastic lifetime

$$\gamma = \frac{\pi\nu_F}{2}(g_4 + g_1), \tag{5}$$

where $\nu_F = -\int d\vec{k}/(4\pi^3)\,\mathrm{Im}\,\mathrm{Tr}\hat{G}(\mu,\vec{k})$ is the density of states (DOS) at the Fermi energy (per spin).

The bulk of the data of Ref. [1] pertains to the metallic regime of relatively high dopings ($\mu > \gamma$), as indicated by the measured mobilities $\sim 10^{4-6}$ cm^2/V s at electron densities $n_e \sim 10^{11-13}$ cm^{-2}, which correspond to $\gamma \sim$ 10–100 K and $\mu \sim$ 100–1000 K. In this regime, the DOS value $\nu_F \approx k_F/(2\pi v_F)$ controlled by a finite radius of the Fermi surface $k_F = \mu/v_F = (4\pi n_e)^{1/2}$ is only weakly affected by disorder.

Under these conditions, the double-pole Green function (4) given by a four-by-four matrix can be well approximated by a pair of two-by-two single-pole matrices representing quasiparticle excitations near the two Dirac points

$$\hat{G}_{1,2}(\omega,\vec{k}) \approx \frac{\hat{1} + \hat{\sigma}_x\cos\phi_k \pm \hat{\sigma}_y\sin\phi_k}{2(\omega - \xi_k + i\gamma)}, \tag{6}$$

where $\xi_k = v_F k - \mu$ and $\phi_k = \tan^{-1}k_y/k_x$.

Also, in the high-density regime, the presence of a large parameter μ/γ facilitates a systematic account of quantum interference corrections to the SCBA results. The leading quantum correction to the zeroth-order (Drude) conductivity is given by the standard single-Cooperon (fan-shaped) diagram. From the technical standpoint, however, a calculation of the corresponding correction appears to be rather involved due to the matrix structure of the Green function (6) and the vertex (2).

The Drude conductivity itself is given by the standard expression $\sigma_0 = (e^2/h)(\Gamma\mu/\gamma)$, where the renormalization factor Γ accounts for a ladder series of vertex corrections associated with one of the two current operators $\vec{J} = v_F(\cos\phi_k, \sin\phi_k)$ inserted into the fermion loop in the diagrammatic representation of the Kubo formula. Being given by a nonsingular (angular momentum $m = 1$) diffusion mode in the expansion over the angular harmonics $e^{im\phi_k}$, Γ is a function of the parameters g_i.

Expanding the full expression for the Cooperon in the same basis as that used in Eq. (2), we obtain equations for the corresponding amplitudes C_i, each of which is a matrix in the direct product of two sublattice subspaces

$$\begin{aligned}
\hat{C}_1 &= g_1\hat{1} + g_2\hat{H}_{12}\hat{C}_1 + g_1\hat{H}_{21}\hat{C}_2,\\
\hat{C}_2 &= g_2\hat{1} + g_2\hat{H}_{12}\hat{C}_2 + g_1\hat{H}_{21}\hat{C}_1,\\
\hat{C}_3 &= g_3\hat{1} + g_4\hat{H}_{11}\hat{C}_3 + g_3\hat{H}_{22}\hat{C}_4,\\
\hat{C}_4 &= g_4\hat{1} + g_4\hat{H}_{11}\hat{C}_4 + g_3\hat{H}_{22}\hat{C}_3.
\end{aligned} \tag{7}$$

Here $\hat{H}_{ij}(\omega,\vec{q}) = \int\frac{d\vec{k}}{(2\pi)^2}\hat{G}_i^R(\epsilon+\omega/2, k+q/2)\otimes\hat{G}_j^A(\omega/2-\epsilon, q/2-k)$ stands for the convolution of a pair of Green functions. Computing it for $\omega, v_F q \ll \gamma$, we obtain

$$\begin{aligned}
\hat{H}_{11,12}(\omega,q) = \hat{H}_{22,21}(\omega,q) = \frac{\pi\nu_F}{4\gamma}\Bigg[&\left(1 + \frac{i\omega}{2\gamma} - \frac{v_F^2q^2}{16\gamma^2}\right)\hat{1}\otimes\hat{1} - \frac{1}{2}\left(1 + \frac{i\omega}{2\gamma} - \frac{v_F^2q^2}{16\gamma^2}\,\frac{3\cos^2\phi_k + \sin^2\phi_k}{4}\right)\hat{\sigma}_x\\
&\otimes\hat{\sigma}_x \mp \frac{1}{2}\left(1 + \frac{i\omega}{2\gamma} - \frac{v_F^2q^2}{16\gamma^2}\,\frac{\cos^2\phi_k + 3\sin^2\phi_k}{4}\right)\hat{\sigma}_y\otimes\hat{\sigma}_y\Bigg].
\end{aligned} \tag{8}$$

It can be readily seen that Eq. (7) splits into two pairs which only couple $\hat{C}_{1,2}$ and $\hat{C}_{3,4}$, respectively. Their solutions read

$$\begin{aligned}
\hat{C}_{1,2}(\omega,q) &= \frac{2\gamma c_{1,2}}{\pi\nu_F}\,\frac{\hat{1}\otimes\hat{1} - \hat{\sigma}_x\otimes\hat{\sigma}_x + \hat{\sigma}_y\otimes\hat{\sigma}_y + \hat{\sigma}_z\otimes\hat{\sigma}_z}{(g_4-g_2)/(g_2+g_1) + v_F^2q^2/16\gamma^2 - i\omega/2\gamma},\\
\hat{C}_{3,4}(\omega,q) &= \frac{2\gamma c_{3,4}}{\pi\nu_F}\,\frac{\hat{1}\otimes\hat{1} - \hat{\sigma}_x\otimes\hat{\sigma}_x - \hat{\sigma}_y\otimes\hat{\sigma}_y - \hat{\sigma}_z\otimes\hat{\sigma}_z}{(g_1-g_3)/(g_3+g_4) + v_F^2q^2/16\gamma^2 - i\omega/2\gamma},
\end{aligned} \tag{9}$$

where

$$c_1 = \frac{g_1^2 + g_1g_4}{(g_4 - g_2 + 2g_1)(g_1+g_2)},\quad c_2 = \frac{g_2g_4 + g_1g_2 - g_2^2 + g_1^2}{(g_4 - g_2 + 2g_1)(g_1+g_2)},\quad c_3 = \frac{g_3g_1 + g_3g_4}{(g_1+g_3)(g_3+g_4)},\quad c_4 = \frac{g_1g_4 + g_3^2}{(g_1+g_3)(g_3+g_4)}. \tag{10}$$

The quantum conductivity correction (including spin) involves the $\hat{C}_1$ and $\hat{C}_4$ components of the Cooperon

$$\delta\sigma(T) = -\frac{e^2}{h}\frac{\pi\nu_F v_F^2}{16\gamma^3}\int\frac{d\vec{q}}{(2\pi)^2}\,\mathrm{Tr}[\hat{C}_1(0,q)+\hat{C}_4(0,q)] \tag{11}$$

whose contributions turn out to be negative and positive, respectively.

At low temperatures, Eq. (11) can be cast in the form

$$\delta\sigma(T) = \frac{2e^2}{\pi h}\ln\frac{\max[\Gamma_\phi/\gamma, |g_4-g_2|/(g_1+g_2)]^{c_1}}{\max[\Gamma_\phi/\gamma, |g_1-g_3|/(g_4+g_3)]^{c_4}} \tag{12}$$

where we introduced an inelastic phase relaxation rate $\Gamma_\phi(T)$ (of either Coulombic or phonon origin, whichever is dominant) providing a finite cutoff in the momentum integration.

The analysis of Eq. (12) reveals that, in the absence of a fine-tuning between the amplitudes of backward scattering and umklapp processes ($g_1 \neq g_3$), the $\hat{C}_4$ Cooperon acquires a gap $\sim\gamma|g_1-g_3|/(g_4+g_3)$. On the other hand, the $\hat{C}_1$ mode remains gapless, provided that all the forward scattering processes are controlled by the same amplitude (i.e., $g_2 = g_4$), which implies the onset of rather conventional weak localization at $T \to 0$.

Conversely, making the C_1 mode gapful and inverting the sign of the conductivity correction would only be possible under the condition $|g_1 - g_3| \ll |g_2 - g_4|$, which is unlikely to be satisfied for any realistic impurity potential that yields equal amplitudes of the processes of intra- and intervalley forward scattering.

Somewhat more generic would be an apparent antilocalizing behavior that can set in at intermediate temperatures, namely, at $\gamma g_1/g_2 < \Gamma_\phi(T) < \gamma$, provided that $g_1 \ll g_2 = g_4$ and $g_3 = 0$ ($c_1 = 1/2$, $c_4 = 1$). At still lower temperatures the overall sign of Eq. (12) would revert to negative, thereby giving rise to a nonmonotonic temperature dependence of the $\ln T$ term in the conductivity.

The above conclusions pertain to the general disorder model (2). However, in the situation where disorder is realized as a random distribution of impurities with a concentration n_i and a (short-range) potential $u(q)$, there are only two independent parameters,

$$g_2 = g_4 = \frac{n_i u^2(0)}{1+[\pi\nu_F u(0)]^2}, \qquad g_1 = g_3 = \frac{n_i u^2(\vec{K}_1-\vec{K}_2)}{1+[\pi\nu_F u(\vec{K}_1-\vec{K}_2)]^2}, \tag{13}$$

which represent the $\hat{T}$ matrix computed for an arbitrary strength of disorder, the customary Born and unitarity (where the scattering phase approaches $\pi/2$) limits corresponding to $u \to 0$ and ∞, respectively. In the case of a genuine long-range (unscreened) impurity potential, a strong momentum dependence of $u(q)$ would make the explicit expressions for g_i more involved, though.

Provided that the relations (13) between the parameters g_i hold, one obtains $c_1 = c_4 = 1/2$, and the logarithmic term in Eq. (12) identically vanishes due to an exact cancellation between the contributions of the localizing ($\hat{C}_1$) and antilocalizing ($\hat{C}_4$) Cooperon modes, thereby resulting in the absence of the leading $\ln T$ correction to the conductivity.

It has to be stressed, however, that the sought-after suppression of (anti)localization would only be possible due to an opening of the umklapp channel. In turn, the latter requires an emergence of a crystal superstructure with the wave vector $2(\vec{K}_1 - \vec{K}_2) = (2/3)(\vec{Q}_1 + \vec{Q}_2)$ or equivalent.

While an isolated sheet of weakly interacting graphene would apparently lack such a superstructure, it is conceivable that the latter could emerge, if a commensurate substrate were used during the process of microfabrication [6]. Alternatively, a commensurate corrugation could occur due to the Coulomb correlations that can induce a spatially periodic pattern of the electron density itself [7]. The possibility of a spontaneous formation of such charge density wave states has long been discussed in the general context of degenerate semimetals and, specifically, in graphene [8].

Next, we contrast our calculations against the arguments presented in Ref. [9] where the possibility of an antilocalizationlike behavior in graphene was originally pointed out. The authors of this work asserted that the equations for the Cooperon mode involve a disorder-induced vertex

$$W_{k,-k,p,-p} = n_i\langle\vec{p}|u|\vec{k}\rangle\langle-\vec{p}|u|-\vec{k}\rangle = n_i u^2(0)e^{i(\phi_k-\phi_p)}[1+\cos(\phi_k-\phi_p)] \tag{14}$$

that makes the full Cooperon amplitude negative for $\vec{k} \approx -\vec{p}$ where $e^{i(\phi_k-\phi_p)} \approx -1$, which fact was claimed to be instrumental for the onset of antilocalizing behavior at $g_1 = g_3 = 0$, although no further technical details were provided.

However, the above argument appears to be invalid, since the actual vertex that ought to be used in the construction of the Cooperon is the particle-hole (exchange) amplitude $W_{k,p,p,k} = n_i\langle\vec{p}|u|\vec{k}\rangle\langle\vec{k}|u|\vec{p}\rangle$, which is given by Eq. (14) without the phase factor in question and which remains non-negative for all $\vec{k}$ and $\vec{p}$.

The true origin of a possible antilocalizing behavior at intermediate temperatures can be traced back to the negative signature of the expansion of the Cooperon mode $\hat{C}_4$ in the product basis $\hat{\sigma}_a \otimes \hat{\sigma}_b$, as opposed to that of $\hat{C}_1$ [see Eq. (9)]. Interpreting the sublattice index as a fictitious spin one-half ($\vec{S}_{1,2} = \vec{\sigma}_{1,2}/2$), one can associate the $\hat{C}_4$ component with the singlet mode $\hat{C}_4 \propto [\hat{1}\otimes\hat{1} - \frac{1}{2}(\vec{S}_1+\vec{S}_2)^2]$, which is known to be a common source of antilocalization in 2DEG with a spin-orbit coupling of the Rashba and/or Dresselhaus kind.

Before concluding, a few more comments are in order. Considering the possibility of the electron density tuning in

the experimental setups of Ref. [1], it would also be of interest to extend the analysis of localization effects to the low-density regime where a finite DOS is dominated by disorder. A similar situation has been previously studied in the context of a normal quasiparticle transport in dirty d-wave superconductors, where $\mu = 0$ and the spectrum possesses an exact particle-hole symmetry [10]. By analogy with that work, for $\mu < \gamma$ one readily finds that the self-consistent DOS and bare conductivity of graphene are given by the expressions $\nu_F \approx (\gamma/2\pi)\ln(v_F/a\gamma)$ and $\sigma_0 \approx 4e^2/\pi h$, respectively.

Unlike in the metallic (high-doping) regime, however, the relative smallness of the quantum conductivity corrections can only be controlled by such a parameter as the (inverse) number of valleys, whose actual value is $N_v = 2$. Moreover, even for an artificially large N_v the calculation of $\delta\sigma(T)/\sigma_0 \sim (1/N_v)\ln[\gamma/\Gamma_\phi(T)]$ involves additional diagrams containing one conventional [made out of one retarded (R) and one advanced (A) Green functions, or "RA"] as well as one anomalous ("RR" or "AA") Cooperon mode, the latter having a small gap $\sim\mu$ [11,12].

Although in the case of dirty d-wave superconductors these new contributions have been argued to reverse the sign of the overall correction to the spin and thermal conductivities [13], we do not find such a behavior in graphene even in the particle-hole symmetrical limit $\mu = 0$, thanks to the formal differences between the Dirac-like descriptions of the two systems. Thus, the aforementioned caveat notwithstanding, our results suggest that the conductivity correction in graphene might retain its sign throughout the entire range of electron densities.

Also, while being the most general model of a random scalar potential due to short-range (screened) impurities, the vertex (2) obviously misses out on those types of disorder that can be best represented by either a random mass of the Dirac fermions or random vector potential. The former might be relevant in the situations where a spatially inhomogeneous charge or spin density wave-type ordering emerges [7,8], whereas the latter describes topological lattice defects (dislocations, disclinations, and cracks) that can be thought of as sources of a random magnetic flux (RMF). The corresponding random vector potential appears to long-range correlated, $\langle \vec{A}_{\vec{q}}\vec{A}_{-\vec{q}}\rangle = 4\pi^2 n_d/q^2$, where n_d is the density of defects.

In an abstract setting, the RMF problem for Dirac fermions has been studied in Ref. [14]. Applying the results of that work, we predict that the RMF-induced elastic scattering gives rise to an additional quasiparticle width $\gamma_d \sim \min[v_F^2 n_d/\mu, v_F n_d^{1/2}]$ [obtaining this result requires one to develop the SCBA for a gauge-invariant counterpart of Eq. (4), since the non-gauge-invariant self-energy (3) diverges with the system size L as $\Sigma_d \propto \sqrt{\ln L}$].

It also follows from the conclusions drawn in Ref. [14] that, in the absence of umklapp, the RMF localization scenario is likely to belong to the so-called "C" universality class [11] which controls the limit $T \to 0$. However, at intermediate temperatures the localization behavior is expected to be governed by a crossover from C to yet another ("A") class [11], due to the predominantly small-angle nature of the RMF scattering.

In summary, we carried out a comprehensive analysis of quantum interference effects in disordered graphene and identified the conditions under which the quantum conductivity correction becomes positive, negative, and zero, respectively. The results of this work provide a further insight into the quantum properties of this novel pseudorelativistic two-dimensional electron system.

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