Effect of weak impurities on electronic properties of graphene: functional renormalization-group analysis

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We consider an effect of weak impurities on electronic properties of graphene within the functional renormalization-group approach. The energy dependences of the electronic self-energy and density of states near the neutrality point are discussed. Depending on the symmetry of the impurities, the electronic damping $\Gamma$ and density of states $\rho$ can deviate substantially from those given by the self-consistent Born approximation. We investigate the crossover from the results of the self-consistent Born approximation, which are valid far from the neutrality point to the strong-coupling (diffusive) regime near the neutrality point. For impurities, which are diagonal in both, valley and sublattice indices, we obtain finite density of states at the Fermi level with the values, which are much bigger than the result of self-consistent Born approximation.

Graphene is a two-dimensional system with the Dirac electronic dispersion, that possesses unique properties. In particular, the electronic properties of graphene near the neutrality point remain a challenging problem of condensed-matter physics. Unlike many two-dimensional systems, the conductivity remains finite at the neutrality point. Although the density of states (DOS) for systems with Dirac dispersion is expected to vanish at the neutrality point, finite DOS at the corresponding position of the Fermi level was observed experimentally in graphene.

The electronic properties of graphene are expected to be strongly influenced by impurities. Although the chiral disorder does not lead to the localization, this particular type of disorder is realized only for infinitely strong impurities (e.g. vacancies). The effect of strong impurities was intensively investigated within both, analytical and numerically exact approaches. Impurities was intensively investigated within both, analytical and numerically exact approaches.

At the same time, even weak impurities may have non-trivial effect on the electronic properties of graphene. In particular, the chiral disorder of the CI symmetry class was argued to yield the energy dependence $e^{1/2}$ of the density of states near the neutrality point. This result is distinctly different from that of the self-consistent Born approximation (SCBA), considering only multiple scattering of electrons on the same impurity, which enlightens the importance of inter-impurity scattering processes. It was also shown in Ref. that for the long-range disorder, which is diagonal in both valley and sublattice spaces, SCBA predicts much smaller damping of electrons close to the neutrality point, than expected from other approaches.

The standard renormalization-group (RG) approach of Ref. allows to describe inter-impurity scattering, but it treats the ballistic regime of the flow only. In particular, this approach yields divergence of the vertices at some critical length scale, which does not allow to describe the crossover to the strong-coupling (diffusive) regime. Investigation of the diffusive regime represents, however, an important problem, since it allows to describe physical properties in the range of fillings close to the neutrality point. Although some results for the density of states and conductivity were obtained within the nonlinear-sigma model approach (see, e.g., Refs. and references therein), it is interesting to perform the analysis starting from the weak-coupling point of view, which may allow to treat both the strong-coupling (diffusive) regime of the flow and the crossover from ballistic to diffusive regime.

In this paper we investigate the effect of long-range and chiral potential impurities on the electronic properties of graphene within the recently proposed Wick-ordered functional renormalization group scheme, allowing to treat self-energy effects beyond the leading order of perturbation theory.

We consider quartic interaction between Dirac fermions due to averaged potential impurity scattering. Assuming only second-order cumulants are important (i.e. the impurity potentials are substantially weak) the corresponding action reads

$$S = \int d^{2}x \left[ \int d\tau \bar{\psi}(\gamma_{\mu}\partial_{\mu})\psi + \frac{1}{2}n_{\text{imp}} \sum_{l} T_{l}^{2} \int d\tau \int d\tau' (\bar{\psi}_{\tau} M_{l} \psi_{\tau'}) (\bar{\psi}_{\tau'} M_{l} \psi_{\tau}) \right]$$

(1)

where $\mu = 0,1,2$, $\partial = (\partial_{\tau}, v_{F}\partial_{x}, v_{F}\partial_{y})$, $\bar{\psi} = \psi^{+}\gamma_{0}$. $\gamma_{\mu}$ are the Dirac matrices, e.g.

$$\gamma_{0} = \begin{pmatrix} \sigma_{3} & 0 \\ 0 & -\sigma_{3} \end{pmatrix}, \quad \gamma_{a} = \begin{pmatrix} \sigma_{a} & 0 \\ 0 & -\sigma_{a} \end{pmatrix},$$

(2)

where $a = 1,2$, $\sigma_{i}$ are the Pauli matrices. The quadratic part of the action represents the continuum limit of the microscopic tight-binding model (see, e.g., Refs. and corresponds to the representation $\psi = \{\psi_{A}^{1}, \psi_{B}^{1}, \psi_{B}^{2}, \psi_{A}^{2}\}$ ($\psi_{a}^{m}$ is an annihilation operator for the electron in valley $m$ and sublattice $s$). The quantities $T_{l}$ represent scattering amplitudes in different channels, characterized by $4 \times 4$ matrices $M_{l}$, which belong to a linearly independent set of complex $4 \times 4$ unitary matrices with $(\gamma_{0}M_{l})^{2} = I$ ($I$ - identity matrix).
The interaction in Eq. (1) is obtained after averaging over impurity positions and potentials \( \{U_i(x_i)\} \) with \( \langle U_i(x)U_j(x') \rangle = n_{\text{imp}}T_i^2\delta(\mathbf{x} - \mathbf{x}') \), \( n_{\text{imp}} \) is the impurity concentration. Eq. (1) neglects higher than second order scattering processes on the same impurity, which implies that this equation is applicable in the limit of weak impurities \( T_i^2/(2\pi v_F^2) \ll 1 \) [1, 13].

The mean-field (self-consistent Born) approximation for the model (1) yields for the fermionic self-energy (see, e.g. Ref. [2] and references therein)

\[
\Sigma(\varepsilon) = -n_{\text{imp}} \sum_{k,i,j} T_i^2 M_i \frac{1}{\gamma_0 \varepsilon - \Sigma(\varepsilon) + i\nu_F \gamma_\alpha k_\alpha} M_j \tag{3}
\]

Taking into account that \( (M_i\gamma_0)^2 = I \), the solution to this equation has the form \( \Sigma(\varepsilon) = \gamma_0 \Sigma(\varepsilon) \) with

\[
\Sigma(\varepsilon) = \frac{U^2 n_{\text{imp}}}{4\pi v_F^2} \left[ \varepsilon - \left( \varepsilon - \frac{(\nu_F \Delta_{\text{uv}})^2}{(\varepsilon - \varepsilon)^2} \right) \right]
\]

where \( U^2 = \sum T_i^2 \), and \( \Delta_{\text{uv}} \) is an ultraviolet momentum cutoff. At \( \varepsilon \to 0 \) equation (4) yields

\[
\Sigma(0) = -i\Gamma; \quad \Gamma \simeq \Delta_{\text{uv}} e^{-2\pi v_F^2/(n_{\text{imp}} U^2)} \tag{5}
\]

Note that exponential smallness of \( \gamma \) in graphene in the limit of weak impurities is due to vanishing of the density of states of pure system at the Fermi level. The density of states of impure system at the Fermi level in SCBA reads

\[
\rho(0) = \frac{4\Gamma}{\pi n_{\text{imp}} U^2} \tag{6}
\]

The renormalization group. To treat the effect of weak impurities beyond SCBA, we apply the recently proposed Wick-ordered functional renormalization-group scheme [11, 12] by considering the sharp momentum cutoff of the electronic propagator in the form

\[
C_\lambda = \left[ \gamma_0 \varepsilon - \hat{\Sigma}_\lambda(\varepsilon) + i\nu_F \gamma_\alpha k_\alpha \right]^{-1} \theta(|k| - \Lambda) \tag{7}
\]

where \( \Lambda \) is the cutoff parameter. The corresponding single-scale propagator reads

\[
S_\lambda = -\hat{C}_\lambda + C_\lambda \hat{\Sigma}_\lambda C_\lambda = \left[ \gamma_0 \varepsilon - \hat{\Sigma}_\lambda(\varepsilon) + i\nu_F \gamma_\alpha k_\alpha \right]^{-1} \delta(|k| - \Lambda), \tag{8}
\]

the dot stands for the derivative over \( \Lambda \). Following Refs. [11, 12], we choose the Wick-ordering propagator in the form, which is complementary to \( C_\lambda \):

\[
D_\lambda = \left[ \gamma_0 \varepsilon - \hat{\Sigma}_\lambda(\varepsilon) + i\nu_F \gamma_\alpha k_\alpha \right]^{-1} \theta(\Lambda - |k|). \tag{9}
\]

In the renormalization-group approach we have contribution of three different channels to the vertex renormalization. The replica trick requires that the diagrams with closed loops (i.e., those containing summations over number of fermion species) should be excluded from the diagram technique. The corresponding RG equation for the vertex \( V_{i_1i_2\ldots i_m}^{\varepsilon\varepsilon'}(k_1, k_2, \ldots, k_3) \), where \( i_m \) and \( k_3 \) correspond to matrix (valley and sublattice) indices and momenta of incoming \((i_1, j_1, k_1, 0)_1\) and outgoing \((i_3, j_3, k_3, 0)_3\) particles, \( \varepsilon \) and \( \varepsilon' \) are the energies of the interacting particles, read

\[
\sum_{ij} V_{i_1i_2\ldots i_m}^{\varepsilon\varepsilon'}(k_1, k_2, k_3) = - \sum_{j} V_{i_1i_2i_4i_4}^{\varepsilon\varepsilon'}(k_1, k + k_3 - k_2, k) V_{i_2i_4i_3i_3}^{\varepsilon\varepsilon'}(k, k, k_3 + k_1 - k_2) \tag{10}
\]

For the self-energy correction we obtain the equation

\[
\Sigma_{i_1i_2\Lambda}(k) = \sum_{p,p',q,q'} V_{i_1i_2i_2i_2}^{\varepsilon\varepsilon'}(k, p, k, k) D_{i_2i_2i_2}^{\varepsilon\varepsilon'}(p) \Sigma_{i_2i_2\Lambda}(p) D_{i_2i_2i_2}^{\varepsilon\varepsilon'}(p)
\]

\[
- \sum_{p,p',q,q'} V_{i_1i_2i_3i_3}^{\varepsilon\varepsilon'}(k, p, q, k) V_{i_1i_2i_3i_3}^{\varepsilon\varepsilon'}(p, k + q - p, q) \times \Sigma_{i_1i_2\Lambda}(p) D_{i_1i_2i_2}^{\varepsilon\varepsilon'}(q) D_{i_1i_2i_2}^{\varepsilon\varepsilon'}(k + q - p) + 2 \text{ perm.} S = \bar{D}. \tag{11}
\]

To solve the equations (9) and (10) numerically we apply the channel decomposition, similar to that proposed in Ref. [14]

\[
V_{i_1i_4}^{\varepsilon\varepsilon',\text{ph}}(k_1, k_2, k_3) = V_{i_1i_4}^{\varepsilon\varepsilon',\text{ph}}(k_3 - k_2) + V_{i_1i_4}^{\varepsilon\varepsilon',\text{ph}}(k_1 - k_3) \tag{12}
\]

expanding vertices \( V_{i_1i_4}^{\varepsilon\varepsilon',\text{ph}}(q) \) (c = ph, ph1, or pp) in harmonics

\[
V_{i_1i_4}^{\varepsilon\varepsilon',\text{ph}}(q) = \sum_{m=0}^{n} \left[ F_{i_1i_4}^{\varepsilon\varepsilon',\text{ph}}(q) \cos(m\varphi_q) + G_{i_1i_4}^{\varepsilon\varepsilon',\text{ph}}(q) \sin(m\varphi_q) \right] \tag{13}
\]

where \( \varphi_q \) is the polar angle of the vector \( q \). Assuming that the disorder is time-inversion invariant, we also use symmetries of the interaction \( V_{i_1i_4}^{\varepsilon\varepsilon',\text{ph}}(q) = T_{i_1i_4} V_{i_1i_4}^{\varepsilon\varepsilon',\text{ph}}(-q) \).
Results. Below we consider the long-range disorder, diagonal in both sublattice and valley subspaces (2 × AI symmetry class), which corresponds to $M_1 = \gamma_0$, $T_i = U\delta_{i,1}$, and one of the chiral disorders preserving time-reversal symmetry $T M_i^T T = M_i$ with matrices $M_i \in \{i\gamma_1, 2i\gamma_3, i\gamma_1, 2i\gamma_5\}$ describing the intervalley scattering of fermions in each of the sublattices $(\gamma_5 = -\gamma_0\gamma_1\gamma_2\gamma_3)$, $T_i = U/2$. The flow for these types of the disorder at the scales $\Lambda \gg |\text{Im} \Sigma|/v_F$, i.e. in the ballistic regime, when one can neglect the quasiparticle damping, was discussed in detail in Ref. [4] (see also references therein). In particular, both disorders, $\gamma_0$ and $i\{\gamma_1, 2\gamma_3, 5\}$ yield the flow of the coupling constants to the strong-coupling regime. For our numerical calculations we use the parameters $U^2 n_{\text{imp}}/v_F^2 = 0.8$, $\Lambda_{\text{uv}} = 2$. The corresponding SCBA damping is $\Gamma = 7.76 \cdot 10^{-4} v_F$. The results of our fRG analysis are presented in Figs. 1-4.

For $\gamma_0$ (long-range diagonal) disorder we find saturation of the density of states and imaginary part of the self-energy at values, which are much larger than the SCBA results (see Fig. 1). This agrees with earlier observation in Ref. [4], that the critical scale of the divergence of vertices in the standard RG analysis $\Lambda_{\text{min}}$ differs from the SCBA result [5] by a factor of 2 in the exponent. The present analysis yields however finite vertices at the critical scale $\Lambda_{\text{min}} \simeq 0.04$ (Fig. 2). The finiteness of the vertices (which divergences are cut at the quasiparticle damping) allows us to describe the crossover between the ballistic ($|\varepsilon| \gg |\text{Im} \Sigma|$) and the diffusive ($|\varepsilon| \ll |\text{Im} \Sigma|$) regimes at the energy $\varepsilon_{\text{cross}} \simeq 0.02v_F \sim \Lambda_{\text{min}}v_F$ and obtain density of states and quasiparticle life-time near the neutrality point. In particular, the quasiparticle damping approaches the value, which is approximately equal to the crossover scale $\varepsilon_{\text{cross}}$.

For $i\{\gamma_1, 2\gamma_3, 5\}$ disorder we find much smaller values of the electronic damping, than for the diagonal disorder. Moreover, at low energies, logarithm of the density of states scales almost linearly with $\ln \varepsilon$, with the slope, which is much smaller, than for SCBA result. The slope of the low-energy region agrees well with that obtained in the strong-coupling analysis of the problem [8], revealing that the density of states is expected to behave as
\( \rho \sim \varepsilon^{1/7} \) at small energies; for the exponent we obtain in the present approach the value 0.1. The values of the maximal vertices, obtained for the considering chiral disorder, are shown in Fig. 4 and grow on approaching neutrality point. This behavior of vertices is similar to the scenario proposed in Ref. [16] for \( d \)-wave superconductors, where it was argued that the diffusons and cooperons in retarded-retarded (RR) channel may show a pole for some symmetries of the disorder. Within the ladder analysis of the problem (similar to that of Ref. [16]), one can show analytically that this scenario is realized for the chiral symmetries of the disorder, provided the singularity exists in the corresponding retarded-advanced cooperons and diffusons [13]. The RG analysis performed here points to a similar situation beyond the ladder approximation. As discussed in Ref. [16], the singularity of the RR diffusons provides peculiarities of the density of states, which is likely related to the observed power law behavior of the DOS for CI symmetry. The results of our study are summarized in the Table.

![Graph showing the density of states for chiral disorder](image)

**FIG. 4:** (Color online) The same as Fig. 2 for chiral disorder of CI symmetry class.

In Conclusion, we have considered the effect of weak impurities on electronic properties of graphene. For long-range disorder, we find saturation of the density of states at the values, which are much bigger than those obtained previously within the SCBA analysis. On the other hand, for chiral impurities of CI symmetry class we find indications of vanishing density of states at the Fermi level, with the power law, which approximates the previously obtained result \( \rho \propto \varepsilon^{1/7} \). The functional renormalization-group approach allows to describe the crossover from the ballistic to the diffusive regime in both cases. For realistic impurities, both long-range and chiral components are present. We expect that long-range component will be dominating in this case. The qualitative behavior of density of states in this case agrees with the recent experimental results [2].

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