Band Structure Transformation as Driving Force Behind Anderson Localization of Charge Carriers in Graphene with Short-range Impurities

Yuriy V. Skrypnyk[1*], Vadim M. Loktev[1,2]

[1]*Bogolyubov Institute for Theoretical Physics, Kyiv, 03143, Ukraine*
[2]*National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute", Kyiv, 03056, Ukraine*

*Corresponding author. Tel: (+38) 0913009109; E-mail: yuriy.v.skrypnyk@gmail.com

The linear dispersion of charge carriers is, undeniably, a visiting card of graphene and is responsible for most of its unique properties. Since the existence of Dirac quasiparticles has been proved for graphene, one of the most intriguing issues of its physics is the possibility of their localization by whichever imperfection that can appear in the honeycomb lattice. Early experiments on graphene-based devices, which were engineered like commonplace field effect transistors, revealed that the sample conductivity never drops below a certain minimum value. This fact, indeed, considerably reduced audacious expectations that corresponding devices are capable of serving as next-generation electronic switches. The minimal conductivity existence has produced quite a stir, and its origin has been relentlessly debated. The Dirac-like dispersion of charge carriers constituted the core of this discussion. The uniqueness of the electron subsystem in graphene was pushed to its limits so much that former physics of semiconductors were sometimes categorically declared being utterly unsuitable for this material. It has been speculated that massless, according to their Dirac dispersion, charge carriers cannot be localized by any degree of disorder caused by lattice imperfections or impurity centers. The presumed impossibility to localize Dirac excitations were directly linked to the minimal conductivity phenomenon. By implementing the method of expanding the averaged Green's function of a disordered system into a series in impurity clusters, we theoretically demonstrate that the electronic band structure of graphene undergoes a qualitative transformation with increasing the impurity concentration. This transformation develops in a threshold manner, is yielded by the significant mutual overlap between individual impurity states in real space, and is manifested by the opening of a transport gap near the Dirac point of the spectrum. We argue that even the simplest model for short-range impurity centers (namely, the Lifshitz one) provides for the Anderson localization of charge carriers in graphene. We determine positions of those spectral intervals, in which electronic states should be localized for a given amount of disorder, and demonstrate that the metal-insulator transition observed in the hydrogenated graphene can be semi-qualitatively described within this approach. Our analytical results are additionally supported by numerical simulations based on the tight-binding model of the impure graphene. Further experiments on functionalized graphene, including the intentional creation of vacancies in its lattice with an accelerated helium ion beam, fluorine deposition, etc. fully confirmed our concept. We predict that certain adsorbates will induce a band structure transformation of the cross type in graphene, which features the doubling of Dirac points in the spectrum, and triggers a possibility to observe the re-entrant metal-insulator transition with varying the Fermi level position.

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