Influence of correlation of impurities on conductivity in graphene

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We present numerical studies of the effect of spatial correlation of impurities on the conductivity of graphene sheets. To calculate electronic and transport properties of graphene we use the real-space time-dependent Kubo–Greenwood formalism within the tight-binding approach, where the diffusion coefficient and conductivity are obtained from the temporal spreading of electron wave packets over the graphene sheets.

The conductance is calculated as a function of the electron density, $\sigma = \sigma(n_e)$, for the cases of random and correlated impurities. To describe both charged impurities on the substrate and neutral adatoms on the graphene sheets, we use the long- and short-range scattering potentials respectively.

The short-range potential is considered in the limiting cases of strong and weak scattering, where the on-site energies respectively $V >> |u|$ and $V \leq |u|$, with u being the hopping energy in the tight-binding Hamiltonian. For the case of the strong scattering ($V >> |u|$) we find that the graphene conductivity is not affected by the spatial correlation of impurities. On the contrary, for the case of the weak impurities ($V \leq |u|$), we demonstrate that the spatial correlation leads to increase the conductivity as the correlation length is increased. Such an effect is similar to that one occurring in conventional solid solutions (alloys). We compare our numerical findings with the corresponding predictions based on the Boltzmann transport equation within the Born approximation and discuss the validity of the latter.

Finally, we study the effect of correlation for the case of the long-range scatterer modeled by the commonly used Gaussian-shaped potential. As for short-range impurities, the long-range Gaussian potential does not lead to any enhancement of the conductivity in comparison to the uncorrelated case.