

Conductivity of graphene and rotated graphene bilayers with point defects

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Electronic transport in graphene is sensitive to static defects that are for example frozen ripples, screened charged impurities, or local defects like vacancies or adsorbates (Refs. [1-4] and Refs. therein). Adsorbates, which can be organic groups or adatoms attached to the surface of graphene, are of particular interest in the context of functionalisation which aims at controlling the electronic properties by attaching atoms or molecules to graphene ([5-7] and Refs. therein). Therefore there is a need for a theory of conductivity in the presence of such defects.

We propose a unified description of transport in one and two graphene sheets with adsorbates that fully takes into account localization effects and loss of electronic coherence due to inelastic processes [10,11]. For the monolayer case, we focus on the role of the scattering properties of the adsorbates and analyse in detail cases with resonant or nonresonant scattering. Sufficiently far from the Dirac energy and at sufficiently small concentrations the semi-classical theory can be a good approximation. Near the Dirac energy we identify different quantum regimes, where the conductivity presents universal behaviours. In rotated graphene bilayers, we analyse in particular the case where defects are in just one layer but affect transport in the other layer due to the interlayer coupling. Numerical results on the role of rotation angle and defects concentration confirm a simple analytical model.

Method

Theoretical studies of transport in the presence of local defects have dealt mainly either with the Bloch-Boltzmann formalism or with self-consistent approximations ([5-10] and Refs. Therein). In these theories a major length scale that characterizes the electron scattering is the elastic mean-free path L_e . These approaches indeed explain some experimental observations but yet these theories have important limitations and can hardly describe in detail the localization phenomena that has been reported in some experiments [4]. Indeed in the presence of a short range potential, such as that produced by local defects the electronic states are localized on the length scale ξ [5-7]. A sample will be insulating unless some source of scattering, like electron-electron or electron-phonon interaction, leads to a loss of the phase coherence on a length scale $L_i < \xi$. Therefore, in addition to the elastic mean-free path L_e the inelastic mean-free path L_i and the localization length ξ play also a fundamental role for the conductivity of graphene with adsorbates.

Here we use a numerical approach for the conductivity that treats exactly the tight-binding Hamiltonian and takes fully into account the effect of Anderson localization. The quantum diffusion evaluate numerically using the MKRT approach [12]. It gives access to the characteristic lengths and to the conductivity as a function of the concentration, the Fermi energy E_F and the inelastic mean-free path L_i [10]. In real samples L_i depends on the temperature, or magnetic field, but it is an adjustable parameter in this work.

Results

Our results confirm that sufficiently far from the Dirac energy E_D and for sufficiently small adsorbates concentrations, the Bloch-Boltzmann theory and the self-consistent theories are valid. Near the Dirac energy we identify different regimes of transport that depend on whether the adsorbates produce resonant or nonresonant scattering. We show also that a proper tight-binding model of graphene which includes hopping beyond the nearest-neighbor leads to sizable modifications of the scattering properties with respect to the mostly used nearest neighbor hopping model.

Some universal aspects of the conductivity are present with or without the hopping beyond nearest neighbors. For small inelastic scattering length L_i such as $L_i \simeq L_e$ the conductivity σ is almost equal to the universal minimum (plateau) of the microscopic conductivity (semi-classical conductivity) $\sigma_M \simeq 4e^2/(\pi h)$ except for $E_F \simeq E_D$ when the model only takes into account nearest neighbor hopping (figure 1). For larger L_i , $L_e < L_i$, the conductivity follows a linear variation with the logarithm of L_i with nearest neighbor hopping only and with hopping beyond nearest neighbors (figure 2). In contrast, the high central peak of the conductivity and the anomalous behavior at the Dirac energy are not robust and are specific to the model with nearest neighbor hopping only. Therefore, we conclude that a precise comparison of conductivity with experiments requires a detailed description of the electronic structure and in particular of that of graphene.

In twisted bilayer graphene, the effective coupling between electronic states of the two layers increases when the angle of rotation decreases, and electronic confinement is obtained for very small angle [13,14,15]. Consequences on transport in twisted bilayer with adsorbates are presented and confirmed by a analytical model.

References

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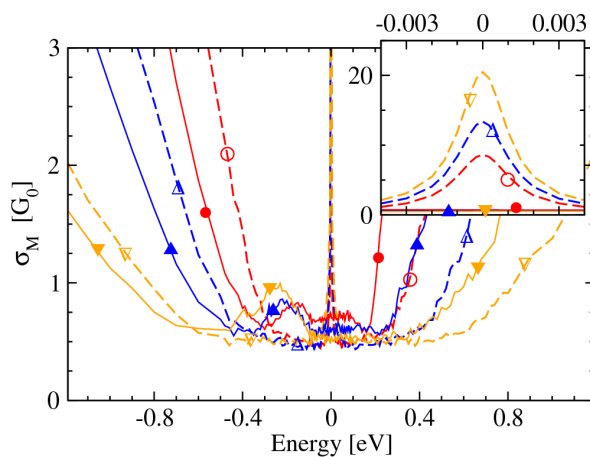


Figure 1: Microscopic conductivity σ versus energy E , for concentration (\bullet) $c = 1\%$, (\blacktriangle) $c = 2\%$ and (\blacktriangledown) $c = 3\%$ of resonant scatters. (dashed line) first neighbor coupling only, (continuous line) beyond first neighbor coupling. $G_0 = 2e^2/h$ [11].

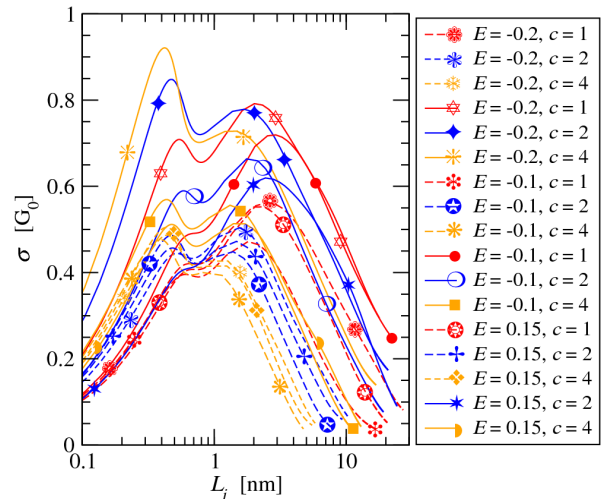


Figure 2: Conductivity σ versus the inelastic scattering length L_i for concentration c (%) and different energies E (eV) in the plateau of $\sigma_M(E)$: (dashed line) first neighbor coupling only, (continuous line) beyond first neighbor coupling [11].