The origin of scattering mechanisms in single- and bilayer graphene

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One of the central issues in graphene research is to identify scatterers that dominate the conductivity σ. This is not only a fundamental question, but also the prerequisite for progress regarding the quality of graphene-based devices for electronics and optoelectronics. Since the character of the scatterers (i.e. long- or short range) manifests itself directly in the dependence of the conductivity σ on the electron density n, this function plays a key role in the corresponding experimental and theoretical investigations.

In most experimental studies the conductivitiy of single layer graphene (SLG) and bilayer graphene (BLG) exhibit similar linear dependences $\sigma \sim n$. The experimental results are commonly analyzed on the basis of the standard Boltzmann approach within the Born approximation. This approach leads to qualitatively different predictions for the short- and long-range scatterers in respectively the SLG and the BLG. This, in its turn, leads to the conclusion that scattering mechanisms has to be different for the SGL and the BLG. This is a rather surprizing conclusion because these mechanisms in both systems are expected to be the same as both the SLG and the BLG are produced by the same manufacturing technique with the same substrate used in the measurements.

Because the conclusions on the nature of scattering mechanisms in graphene rely essentially on the predictions of the Boltzmann approach, it is of the utmost importance to establish the limits of its validity for the SLG and the BLG. In the present study we first derive analytical expressions for the conductivity of the SLG and the BLG within the standard Boltzmann approach for the Gaussian disorder and then compare them with the exact numerical tigth-binding (TB) Landauer-type calculations.

(a) SLG [1]. We demonstrate that for the SLG the TB calculations give the same linear density dependence of the conductivity, $\sigma^{TB} \sim n$, for short- and long-range Gaussian scatterers. In the case of short-range scattering the TB calculations are in agreement with the predictions of the Boltzmann theory going beyond the Born approximation but in qualitative and quantitative disagreement with the standard Boltzmann approach within the Born approximation predicting $\sigma^{Boltz} \sim$ const. Even for the long-range Gaussian potential the standard Boltzmann predictions are in quantitative and qualitative disagreement with the TB results in a parameter range corresponding to realistic systems, $\pi n\xi^2 << 1$ (with ξ being the effective screening length of the Gaussian potential). This questions the validity of the standard Boltzmann approach within the Born approximation, commonly used for the interpretation of the results of experimental studies of the conductivity in the SLG [1].

(b) BLG [2]. For the case of BLG we demonstrate that, as for the case of SLG, the standard Boltzmann approach and the TB calculations agree qualitatively and quantitatively in the regime of $\pi n\xi^2 >> 1$ (corresponding to high densities/smooth potential). This regime however is not achieved in realistic devices. In the opposite regime $\pi n\xi^2 <<1$ appropriate to all experiments, our findings are strikingly different from those for the case of SLG where the Boltzmann approach is not valid. We find that for the

BLG the Boltzmann approach is consistent with the corresponding TB calculations for the range of electron densities where the BLG dispersion is parabolic. In this regime the Boltzmann theory predicts $\sigma \sim n$ regardless of the potential range ξ (i.e. for both short- and long-range Gaussian potential), which is confirmed by the TB calculations in the parameter range of ξ explored in our study. For higher electron densities when the BLG dispersion is linear, the Boltzmann and the TB calculations disagree.

References

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