Effective contact model for geometry-independent conductance calculations in graphene

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Abstract The starting point of any calculation of quantum conductance in the Landauer-Büttiker formalism using Green's functions (GF) is Caroli's formula. This formula has been extensively used for nanoribbons geometries, but the only restriction about the geometry of the nanostructure is the GF of the contacts. As far as we know, this is the first attempt to adapt the GF’s method to a Corbino disk geometry. Our method assumes that the contact is an $s$ band metal and that its DOS is nearly constant at the Fermi Energy; based on these an effective self-energy term is introduced in the GF’s calculation of the quantum conductance [1]. When compared with the results obtained by Dirac’s equation [2] our calculations agrees with the conductance obtained via the Dirac equation ($G_D$) irrespective of the geometric parameters like inner radius ($R_i$) and outer radius ($R_o$), as can be seen in Fig. 1 where the normalized conductance is shown as a function of the Fermi energy in the annulus region for $R/R_o=0.007, 0.86, 0.47$. This range of geometric parameters was chosen to analyze the effect of the disk size (number of atoms) on the conductance, and also to allow us to probe the effect of varying the number of edge atoms (atoms with on-site energy modified by the effective self-energy term). Surprisingly the conductance as a function of energy doesn’t show plateaus for the total angular momentum eigen-channels, being characterized only by Fabry-Perot oscillations that are more prominent in our model because of the roughness of the metal-graphene interface. For wide disks the conductance at the Dirac point is reduced but never reaches zero, as would be expected in a semi-classical calculation, due to the influence of evanescent states. Evanescent states are also responsible for higher values of conductance for larger inner radii, since more total angular momentum eigen-channels are allowed to transmit. Our model reproduces the magneto-conductance characteristics of a Corbino disk as well. The advantage of GF’s methods is the possibility of introducing disorder, which we explore and characterize by adding short-range onsite disorder (Anderson type) in order to calculate the radial part of the conductivity tensor ($\sigma_{rr}$).

References

[1] D. A. Bahamon, A. H. Castro Neto and Vitor M. Pereira, *Phys. Rev. B*, 88 (2013) 235433

[2] A. Rycerz, P. Recher and M. Wimmer, *Phys. Rev. B*, 80 (2009) 125417

Figures
Figure 1. Energy dependence of the conductance normalized by $R_i$ for different values of $R_i$ and $R_o$, calculated using Dirac equation (labeled "D") and the lattice Green's function approach (labeled "G"). The inset shows the relative differences in the values of conductance calculated by the two methods $\Delta G = 100(G_G - G_D)/G_D$. 