Electronic transport in graphene-based structures: An effective cross section approach

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We show that transport in low-dimensional carbon structures with finite concentrations of scatterers can be modeled by utilising scaling theory and effective cross sections [1]. Our reults are based on large scale numerical simulations of carbon nanotubes and graphene nanoribbons, using a tight-binding model with parameters obtained from first principles electronic structure calculations. As shown by a comprehensive statistical analysis, the scattering cross sections can be used to estimate the conductance of a quasi-1D system both in the Ohmic and localized regimes. They can be computed with good accuracy from the transmission functions of single defects, greatly reducing the computational cost and paving the way towards using first principles methods to evaluate the conductance of mesoscopic systems, consisting of millions of atoms.

[1] A. Uppstu, K. Saloriutta, A. Harju, M. Puska and A.-P. Jauho, arXiv:1111.0148v1