Conductance distributions in doped single wall Carbon nanotubes: full ab-initio calculations versus macroscopic models.

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In low dimensional systems, the effect of coherent multiple scattering of charge carriers plays a crucial role in transport properties[1]. The disorder inherent to many systems leads to fascinating statistical transport properties, such as Universal Conductance Fluctuations (UCF) [2] or Anderson Localization [3]. Different statistical descriptions of electronic transport through low dimensional systems have evolved over time.

On the one hand, macroscopic approaches, often based on random matrix theory (RMT) [4], consider the scattering matrix of the system as an statistical variable from which relevant transport coefficients can be obtained through the use of Landauer-Büttiker formalism for two probe systems. One of the most celebrated such theoretical frameworks is the DMPK equation [5], it describes the evolution of transport coefficients statistics as a function of the system length. In DMPK, all statistical transport properties depend on a single scaling parameter, namely the length of the system normalized by the transport mean free path.

On the other hand, accurate and realistic first principle models have acquired enough efficiency to deal with large systems. For instance, calculations of conductance as a function of energy, length and functional groups concentration in functionalized single wall carbon nanotubes (SWCNT) [6] can be performed up to micrometer lengths and coverages of hundreds of functional groups.

Only recently both theoretical approaches has been partially compared for rather realistic systems. For instance in [7], first principles modeling of transport through doped Silicon nanowires has confirmed the one-parameter scaling hypothesis comparing conductance averages, and its fluctuations, as a function of system length in the diffusive regime.

Nevertheless, several questions are still open. It is known [8] that surface and bulk disorder can lead to different shapes in the statistical conductance distributions even though they present similar behavior of the first moments of the distribution in the diffusive regime. The comparison of the above mentioned theoretical descriptions all the way from the quasi-balistic regime to the deep localized one has not been done. Interestingly, If the system under consideration is a SWCNT with some kind of scattering sources, it is not clear whether the statistical signatures of disorder will correspond to surface or bulk disorder. It is the purpose of this work shedding light on these questions.

To do so, we study charge transport through metallic SWCNT's with random distribution of phenyl groups attached to the tube surface. The attachment of this functional groups allows us to introduce a defect in the surface of the nanotubes which has consequences in the potential distribution around the grafting sites. Our results describe how the nanotube conductance is perturbed as a function of incident electron energy and functional groups coverage density. To cope with this task an efficient numerical method is crucial. We use a hybrid scheme where we resort to both first principles calculations, to obtain a suitable parametrization of the electronic structure, and a real space renormalization procedure to reduce the size of the system and, then, to solve for the transport problem of large and disordered systems [6]. The quantum transport modeling is based on the Green's function formalism, combining an

iterative scheme for the calculation of transmission coeficients with the Landauer-Büttiker formula for the coherent conductance.

We then compare the results obtained by first-principles calculations with the DMPK equation predictions. The input parameters for the DMPK equation are the number of channels, two in the case of a SWCN, and its average conductance. Using these data we perform a Monte Carlo integration of the joint probability distribution function of the transport eigenvalues in order to obtain the conductance distribution for the current ensemble of functionalized SWCN's.

In Fig.1 we compare both first-principles and DMPK conductance distributions. It can be seen that the full conductance distributions coincide to a large extent within the numerical accuracy of DFT calculations. Furthermore it can be shown that this agreement remains valid at all transport regimes, from quasi-balistic to localized ones.

This fact implies that transport in doped SWCN's is controlled by a single scaling parameter (the averaged conductance) and that the macroscopic transport properties can be obtained through the properties of a single scatterer. Hence, these properties can be predicted for arbitrarily large systems.

On the other hand, the validity of the DMPK signals the bulk nature of the scattering induced by disorder in contrast to surface disorder.

It is worth emphasizing that there is no fitting parameter, the whole conductance distributions are obtained once the average value is fixed.

This quantitative agreement between DMKP and ab-initio descriptions might be extended to more comprehensive descriptions based on RMT [9] able to describe systems where bulk and surface disorder play different roles [10].

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Figures

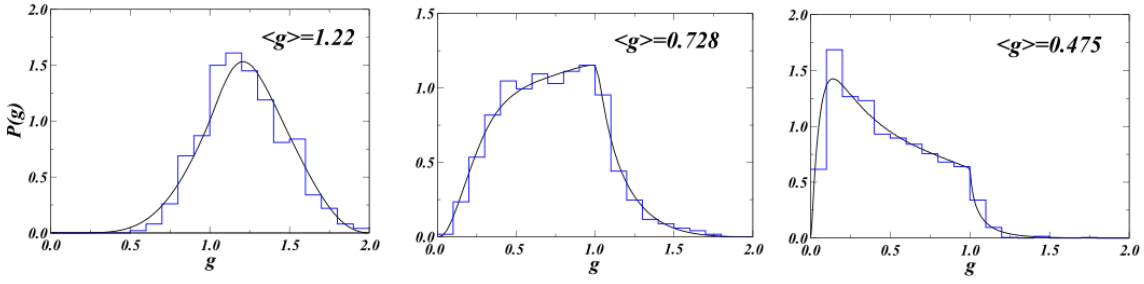

Figure 1: Conductance distributions for different ensembles of functionalized SWCNT's labeled by its averaged conductance. Histograms corresponds to DFT simulations and lines to the DMPK distributions.