Interpolation scheme to speed up *k*-point averaging: applications to graphene structures

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Abstract
Calculations of electronic conductance based on first principle methods provide a parameter-free route to assessing the scattering properties of extended defects in graphene such as grain boundaries [1] or adsorbate structures [2]. Typically these are treated employing periodic boundary conditions in the direction transverse to the transport direction and a corresponding *k*-point average. This means that for each *k*-point the system essentially behaves as a one-dimensional conductor with diverging density of states and discontinuities in the transmission function at energies corresponding to band on-sets/channel openings. It is well known that in order to obtain smooth and converged DOS and transmissions as a function of energy a substantial number of transverse *k*-points are needed due to the rapid variations of the functions for individual *k*-points. This can amount to a significant computational burden for large systems treated by first principle methods such as DFT-NEGF.

Here we present a simple and efficient interpolation scheme which can significantly speed up the convergence with *k*-points of DOS and transmission calculations through nanostructured systems.

Calculations are performed using the software package SIESTA, which implements density functional theory using localized basis sets [3]. The extensions TranSIESTA and TBTrans allow us to calculate the ballistic transport through a device region when electrodes have been defined [4]. We use an accurate DZP basis (13 orbitals per carbon atom) with a *k*-grid that ensures relative convergence in energy. The electrodes are made semi-infinite by adding self-energies, and the amount of transverse *k*-points is varied to check convergence.

We apply our interpolation scheme to several test cases: (i) pristine graphene (see Fig. 1a), (ii) graphene with hydrogenation along a line ("kinked graphene") [2] (see Fig. 1b), and (iii) graphene nano-constrictions [5]. The three mentioned cases show the diversity and generality of the interpolation scheme, and its potential to reduce computation time. The outcome is shown in Fig. 2. Finally, we will address the intrinsic limitations of the scheme.

References
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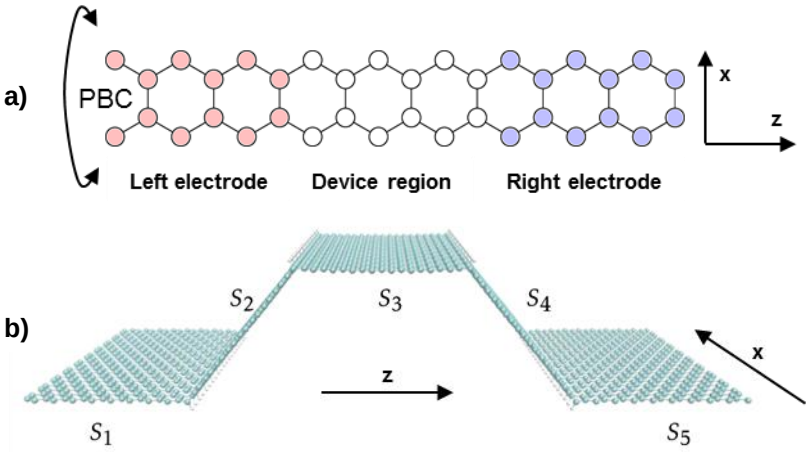

Figure 1: *Considered systems: (a) pristine graphene, and (b) hydrogenated graphene along lines ("kinked graphene"). Both structures have periodic boundary conditions in x while the transmission is calculated along the z-axis.*

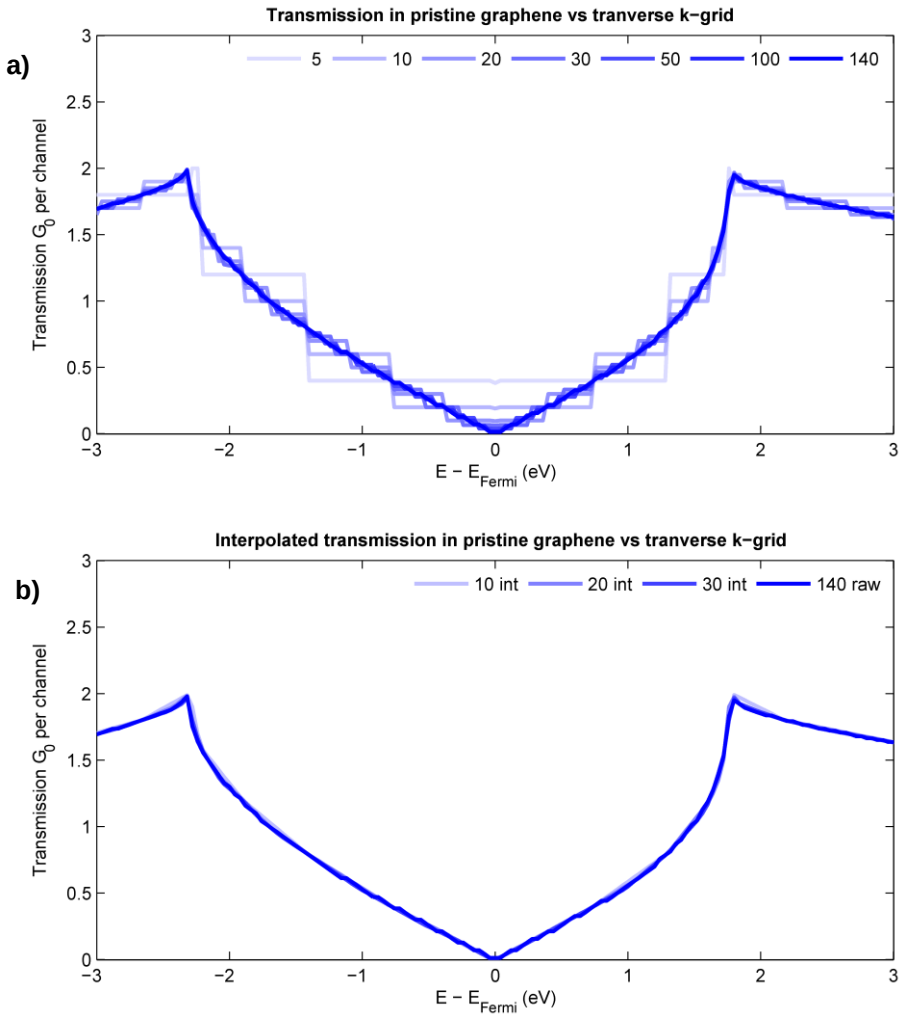

Figure 2: *(a) Transport through pristine graphene from left (red in Fig. 1a) to right electrode (blue in Fig. 1a) as a function of number of transverse k-points. (b) The interpolated transmission in pristine graphene shows much faster convergence.*