Role of zero-energy modes in low energy quantum transport through disordered graphene

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The interplay between disorder and symmetry in driving quantum transport at the Dirac point of graphene is a highly debated subject of fundamental interest, whose investigation represents a theoretical and experimental challenge. Of particular importance is the case of resonant scatterers, i.e. short-range defects giving rise to resonant states, typically at low energy.

The theoretical and numerical studies on this subject have mainly focused on the case of pseudo-vacancy disorder, for which the orbitals corresponding to the missing atoms are simply removed from the tight-binding Hamiltonian of the system. This type of disorder represent a wide class of defects for which the hybridization of the carbon atoms passes from sp^2 to sp^3, as for example in the case of hydrogen adsorbates. We consider pseudo-vacancies homogeneously distributed over the two sublattices of graphene (compensated case) or only over a single lattice (uncompensated case). The main results of the literature predict that: (i) uncompensated vacancies induce very localized zero-energy states and reduce the density-of-states around the Dirac point thus opening a gap [1]; (ii) compensated vacancies at exactly the Dirac point give rise to a *supermetallic* state that makes the minimum conductivity rise above $4e^2/h\pi$ when increasing the defect density [2]; (iii) for uncompensated vacancies the conductivity increase is rapidly suppressed even for very low defect densities [2].

In this contribution [3], we get to the heart of the issue by simulating electronic transport through graphene in the presence of compensated and uncompensated vacancies at low energies around the Dirac point. To this aim, we consider two different and complimentary system configurations: 2D graphene (investigated by the Kubo-Greenwood approach) and graphene strips with high aspect ratio in between two highly doped contacts (for which we made use of the Green's function technique), see Fig.1.

In the case of uncompensated vacancies (Fig.2), both configurations show the opening of a band gap that increases as the square root of the defect density and leads to conductivity suppression. Very close to the Dirac point, a conductivity peak unveils the presence of very localized zero-energy states, whose contribution to transport is however almost irrelevant, as we will explain.

Compensated vacancies globally preserve the sublattice symmetry, thus entailing a completely different conductivity behavior. For 2D graphene, the semiclassical conductivity at the Dirac point shows a marked peak above $4e^2/h\pi$, which is consequence of the important contribution of the induced zero-energy modes, see Fig.3(a). However, the effect of Anderson localization is evident from the quantum conductivity, which turns out to be progressively reduced for long quantum coherence times. In the case of the graphene strip, where transport is dominated by tunneling through the undoped region, the conductivity shows a peak close to the Dirac point, see Fig.3(b). The peak height (averaged over several disorder realizations) is found to be a universal function of the vacancy density times the square of the strip length. For very low values of this parameter, the peak fluctuates around $4e^2/h\pi$ and can be occasionally higher for specific disordered realizations. This is a signature of the competing effects of the low-energy increase of the density-of-states due to the zero-energy modes and the scattering due to the disordered distribution of the defects. When increasing the density, the conductivity peak decreases logarithmically, thus evidencing the progressively dominant role of scattering.

Our results provide a broad numerical perspective on this interesting problem and clarify the interplay between sublattice symmetry and transport at the Dirac point, thus giving a possible explanation of the observed Anderson localization in ultraclean samples [4].

References

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Figures

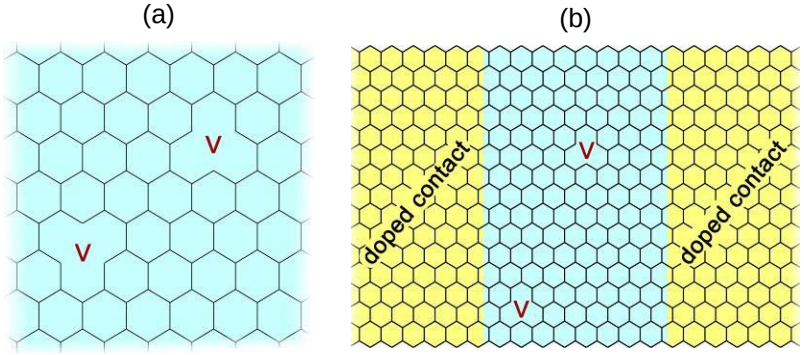

Figure 1: (a) Two-dimensional graphene with two pseudo-vacancies indicated by the letter V. (b) Strip configuration composed of a graphene strip with high aspect ratio (width *W* much larger than length *L*) between two highly doped contacts. Transport occurs by electron tunnelling through the undoped region.

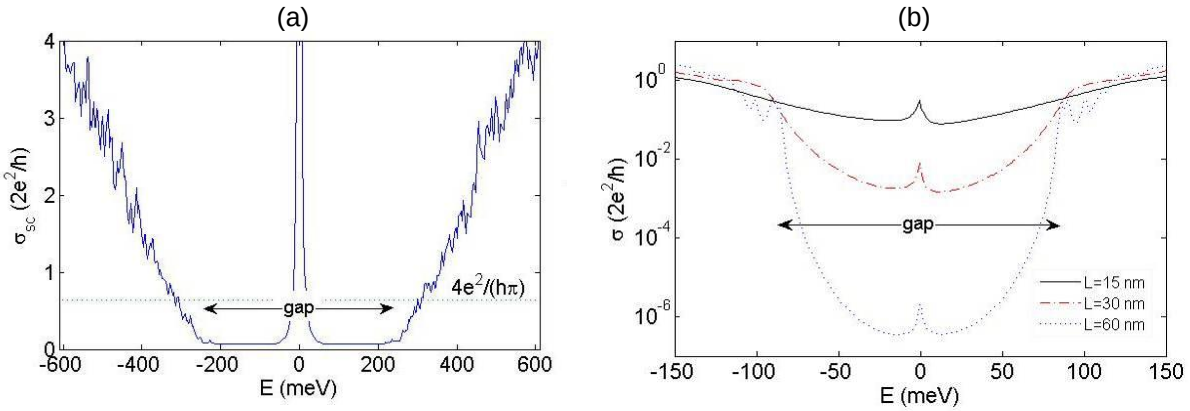

Figure 2: (a) Semiclassical conductivity as a function of energy in 2D graphene with uncompensated vacancy density *n*=0.8%. (b) Quantum conductivity as a function of energy for a strip with *W*=150 nm, different lengths *L* and uncompensated vacancies with density *n*=0.1%.

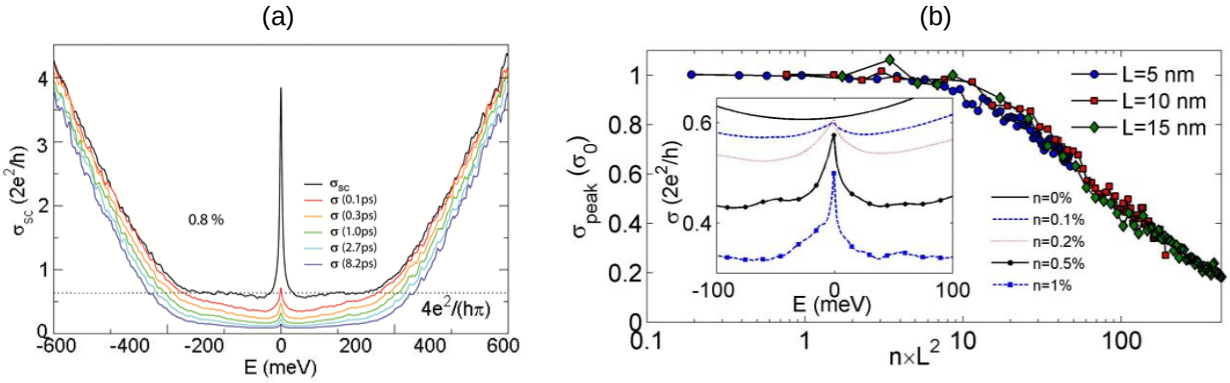

Figure 3: (a) Semiclassical (σ_{SC}) and quantum (σ) conductivity for 2D graphene with density of compensated vacancies *n*=0.8%. Note that the peak at the Dirac point is progressively suppressed due to localization effects. (b) Inset: Average conductivity (over 20 disorder realizations) as a function of the energy for a strip with width *W*=150 nm, length *L*=5 nm and compensated vacancies with density up to *n*=2%. Note the peak at *E*=0. Main frame: Height of the conductivity peak as a function of nxL^2. The conductivity fluctuates around the pristine minimum conductivity as long as of $nxL^2<10$, then it decreases.