Localization of states on graphene-type lattices

C. González-Santander[1], F. Domínguez-Adame[1], R. A. Römer[2]

[1] GISC, Departamento de Física de Materiales, Universidad Complutense de Madrid, E-28040, Spain
[2] Department of Physics and Centre for Scientific Computing, University of Warwick, Coventry, CV4 7AL, United Kingdom

cglezsantander@fis.ucm.es

Abstract

The electronic properties of charged particles in two-dimensional (2D) systems under arbitrary disorder have attracted much attention in the last years. Not only from the theoretical point of view, because the scaling theory predicts that all states are localized in 2D, but also whether there are experimentally achievable true 2D systems. Graphene has been proposed as the most suitable material to address these questions [1-4]. Most of the numerical studies claim that, as expected, disorder induces localization in graphene. The detailed features of the localized behaviour depend on the precise numerical approaches employed for evaluating, e.g. the single-particle wavefunctions or the conductivity of the graphene samples. A few papers even propose that graphene can support a localized to extended transition [3,4]. Therefore, the problem of localization in 2D systems, and specifically in graphene, is still under debate and resembles somewhat the discussion of 2D localization of the mid 1980's.

In this work we proposed a novel approach based on a combination of the transfer matrix method and the power method for diagonalizing Hermitian matrices. Our methods allows to study 2D samples of size MxM directly without having to use quasi-1D geometries. We apply the method to both a simple square lattice (SQ) and a hexagonal lattice, representing a graphene sample, with zigzag (ZZ) and armchair (AC) edges. Our calculation is based on the Anderson tight-binding Hamiltonian for an electron in a lattice with compositional disorder. The on-site potentials are randomly distributed according to a uniform distribution with width W.

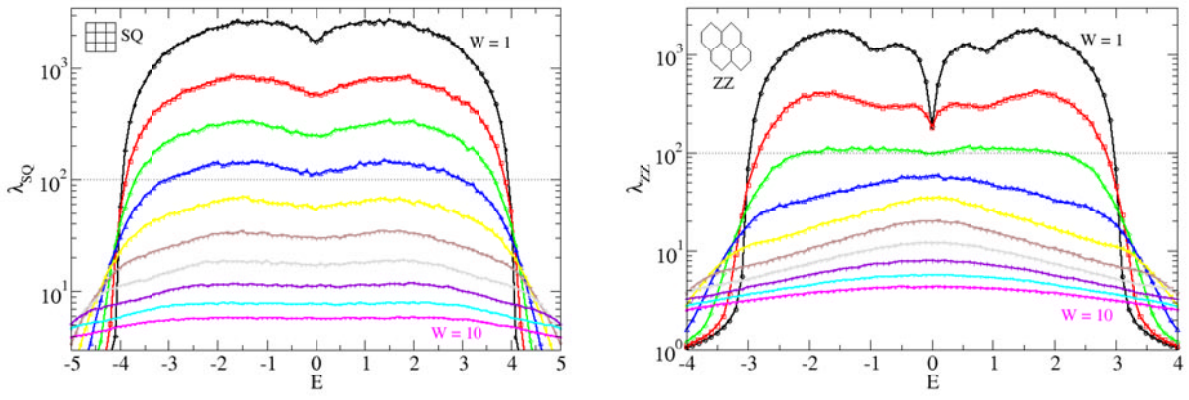
Fig. 1 shows the localization lengths λ for (a) SQ and (b) ZZ lattices as a function of energy, E, for different disorders, W, ranging from W=1 to 10, for systems with 10^4 lattice sites. Results have a relative error equal or smaller than 2.5%, which is obtained averaging over at least 500 disorder configurations. For comparison it should be noted that all lengths are given in units of the nearest neighbour distance, and therefore is different for each lattice, according to its topology. When the strength of the disorder increases the localization length found to decrease as expected because the wavefunctions become more localized. This effect is so robust that under strong disorder the localizations lengths are one order of magnitude smaller than the system size. However, for weaker disorders the localization lengths are bigger than the system size. Hence these states appear as extended, when actually this is a finite size effect.

A truly localized to extended transition can be studied from the dependence of the reduced localization length $\Lambda=\lambda/M$ on the width M. In the localized regime Λ decreases with M since λ remains finite in the thermodynamic limit. On the other hand, Λ increases for extended states. At the transition Λ is constant. In order to describe a system with infinite width and length it is necessary to extrapolate the computed data of λ with M. This can be done through a finite size scaling (FSS) procedure [5], assuming that $\Lambda=f(\xi/M)$ where ξ is the scaling parameter. In Fig. 2 Λ is plotted as a function of ξ/M for (a) SQ and (b) ZZ lattice at E=0. Results show that it is possible within the accuracy of our data to find a scaling function with only the localized branch. Even more, the SQ and ZZ data can be combined into a single such localized FSS curve. The presence of this one branch is a sign of the complete localization of states for large systems and hence the absence of an Anderson transition. Similar results are obtained for AC graphene-type lattice.

References

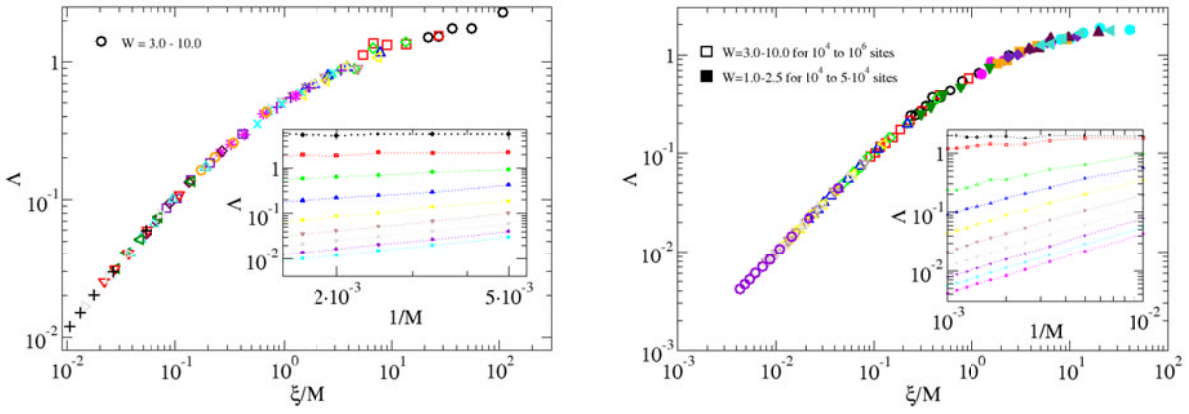
[1] S.-J. Xiong and Y. Xiong Physical Review B, **76** (2007) 214204.
[2] G. Scubert, J. Schleede and H. Fehske Physical Review B, **79** (2009) 235116.
[3] M. Amini, S. A. Jafari and F. Shahbazi EPL, **87** (2009) 37002.
[4] M. Hilke arXiv:0912.0769v1 (2009)
[5] A. MacKinnon and B. Kramer, Z. Phys. B – Condensed Matter, **53** (1983) 1.

Figures



(a) **(b)**

Figure 1. Localization length λ as a function of energy *E* for (a) SQ and (b) ZZ lattices for systems with 10^4 lattice sites for different disorders *W* from *W*=1 to 10 in steps of 1. Only the labels for *W*=1 and *W*=10 are indicated for simplicity. The size of the plotted symbols are within the error bars. The width of the sample *M*=100 is indicated by a dotted line.



(a) **(b)**

Figure 2. Reduced localization length Λ as a function of ξ/*M* for (a) SQ and (b) ZZ lattices for systems from 10^4 to 10^6 lattice sites for different disorders W from *W*=1 to 10 at *E*=0. Insert shows Λ as a function of 1/*M*.

Acknowledgments

The numerical calculations haven been done at the Centre for Scientific Computing at the University of Warwick, England and the Centro Nacional de Supercomputación (BSC – CNS), España.