Coulomb Edge Effects in Graphene Nanoribbons

W. Jaskólski¹ and A. Ayuela²

¹ Instytut Fizyki, Uniwersytet Mikołaja Kopernika, Toruń, Poland ² Centro de Fisica de Materiales CFM-MPC CSIC-UPV/EHU and Donostia International Physics Center, San Sebsatian, Spain

Graphene has become recently the most intensively studied material in condensed matter physics and in material sciences. This is because of its unusual transport and magnetic properties which are expected to find applications in novel nano-electronic devices. Such applications require the usage of nanosize structures of graphene, like graphene nanoribbons (GNR) and quantum dots, in which the properties of edges may be dominant. Graphene ribbons exhibit edge-localized electronic states with energies close to the Fermi level [1], which play a crucial role in transport and magnetic properties of GNRs. The edge-localized states are especially sensitive for the electron-electron interaction effects. However, the role of the Coulomb effects has been so far studied mainly for the zigzag and Klein-like edges. Here, we investigate the influence of Coulomb effects on the edge localized states of chiral GNRs with arbitrary shape of the edges. We employ a π -electron tight-binding approximation, and the electron interaction effects are included by the Hubbard model.

It was recently shown that chiral ribbons with the so called minimal edges, based on translation vector (n,m), have similar zero-energy band structure as pure zigzag ribbons (n-m,0). Here we show that flat, edge-localized bands with energies at the Fermi level are, in fact, different in both cases. The bands of chiral ribbons are non-degenerate, they split at the values of wavevector, for which the bands of (n-m,0) zigzag ribbons are degenerate. We demonstrate that Coulomb interaction enhances strongly the splitting. Spin degeneracy is further lifted when the edges are non-minimal. It happens even when there is no sublattice imbalance in the ribbon unit cell. The strengths of the splitting depends on the edge modification and in some cases leads to spin-filter transport properties of the ribbons. It concerns also quantum dots built of finite fragments of GNRs. In quantum dots, the flat bands close to the Fermi level reduce to a set of discrete spin-polarized states. The corresponding wavefunctions are localized at the GNR edges, so they can yield not only the spin-polarized but also the edge-localized transport.

[1] W. Jaskólski, A.Ayuela, M. Pelc, H. Santos, and L. Chico, Phys. Rev. B. 83, 235424 (2011)