Edge states and flat bands in graphene nanoribbons with arbitrary geometries

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We prescribe general rules to predict the existence of edge states and zero-energy flat bands in graphene nanoribbons and graphene edges of arbitrary shape. [1] No calculations are needed. For the so-called *minimal* edges, the projection of the edge translation vector into the zigzag direction of graphene uniquely determines the edge bands. By adding nodes to minimal edges, arbitrary modified edges can be obtained; their corresponding edge bands can be found by applying hybridization rules of the extra states with those belonging to the original edge. Our prescription correctly predicts the localization and degeneracy of the zero-energy bands at one of the graphene sublattices, confirmed by tight-binding and first-principles calculations. It also allows us to qualitatively predict the existence of $E\neq 0$ bands appearing in the energy gap of certain edges and nanoribbons.

We also apply these rules to graphene nanoribbons and carbon nanotubes containing ordered defect lines built of octagonal rings.[2] We show that octagonal defect lines are a robust source of state localization at the Fermi energy, in some cases leading to spontaneous magnetization. We also prove that the localization at chains of octagons is a consequence of the zigzag nature of the graphene edges forming the defect lines.

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

[2] M. Pelc, L. Chico, A. Ayuela, and W. Jaskólski, Phys. Rev. B **87**, 165427(2013).