Graphene edge states characterization by a new numerical tool: Edge Fraction

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Abstract

We propose a numerical method for identification and analysis of edge states in two dimensional lattices, through computing what we called the Edge Fraction of each electronic state of the system, a quantity that gives the proportion of the total wave function that is concentrated at an specified width at the edges. Here we apply this method to investigate details of edge states from graphene finite lattices with sharp zigzag and armchair edges. Computing the Edge Fraction of states for graphene systems in the quantum Hall regime, we clearly identify the edge states between the Landau levels (LL), observing differences on the edge localization properties depending on the LL index, and on disorder. If the quantity is calculated separately for each edge type, it allows one to distinguish the circulating quantum Hall edge states (equally distributed over the edges) from localized wave functions at only one edge type. We observe well defined energy windows at the threshold of the n =0 and n =1 Landau levels, for which the edge states are predominantly over zigzag or armchair edges, respectively (Figure 1). Signatures of these zigzag and armchair localized edge states in energy vs magnetic field spectra are observed and analyzed, helping in understanding the evolution of edge states with magnetic field and to elucidate details of these spectra. Edge Fraction is also shown to be a useful tool to analyze edge states in absence of magnetic field.

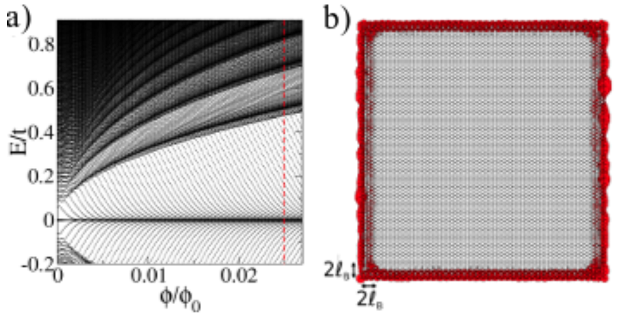

Figure 1: a) Energy spectrum as a function of magnetic flux for a graphene lattice with sharp zigzag and armchair edges, showing the formation of Landau levels with square root energy dependence on magnetic field and the n = 0 level at E = 0. b) Probability density distribution for the state pointed by the red arrow in a). The state is clearly an edge state, with densities concentrated within the distance $2l_B$ from the edges. The graphene lattice size considered here is 17nm x17nm.