Broken Translation Symmetry and Edge States

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The successive miniaturization of graphene-based electronic devices has triggered a broad interest in edge states that essentially influence the electronic band structure and electronic transport properties of nanometer-sized samples (see, for instance [1] and references there). The appearance and properties of these localized states depend sensitively on microscopic details of the edge, particularly these properties depend on the orientation of the edge in respect to the primitive vectors of the lattice like different so called zigzag and armchair edges in graphene. The mathematical description of the edge states is more complicated as compared with the bulk states because the edge breaks some translation symmetries, and this breaking is different for the above mentioned different edges. This feature isn't the prerogative of the particular graphene lattice but is inherent to any other lattice if the microscopic structure of it is taken into account.

The purpose of the present report is to illustrate the interplay of the above mentioned translation symmetry breaking and the particular properties of the edge states making use of the simplest model square lattice. In the case of the most symmetric edge (when its direction coincides with the primitive vector) we used the translation along the edge symmetry for transforming the two dimensional (2D) tight binding method equations to more simple 1D eigenvalue problem. The exact solution of the latter one was obtained by means of the Bethe's Ansatz which was checked by the numerical diagonalization. When the direction of the edge doesn't coincide with primitive vector the above mentioned symmetry is broken. Nevertheless it can be restored enlarging the primitive cell and the number of wave function components, what enables to use the above procedure. The edge state appears in the case when there is a force that keeps the electron close to the edge. The role of this force can be played by the additional local potential of atoms at the edge, or the modified electron tunneling amplitude along it. The influence of both these factors to the edge state properties is studied and the relation of them to the broken translation symmetry is traced. Thus, in the case of most symmetric edge the electron motion along it changes the effective local potential, and consequently, the edge state energy shift depends essentially on electron momentum along the edge, while in the less symmetric edge case the local potential and tunneling amplitude acts in a similar way.

[1] K. Wakabayashi et al, Sci. Technol. Adv. Mater. 11, 054504 (2010).