Accepted Manuscript

Study of simulated Bloch oscillations in strained graphene using neural networks

J.A. González, C.E. López, A. Raya

PII: S2352-2143(18)30218-1

DOI: 10.1016/j.cocom.2018.e00326

Article Number: e00326

Reference: COCOM 326

To appear in: *Computational Condensed Matter*

Received Date: 13 July 2018

Revised Date: 8 August 2018

Accepted Date: 8 August 2018

Study of simulated Bloch oscillations in strained graphene using neural networks.

J A González[a], C E López[a], A Raya[a]

[a]*Laboratorio de Inteligencia Artificial y Supercómputo, Instituto de Física y Matemáticas, Universidad Michoacana de San Nicolás de Hidalgo, Morelia, 58040, México*

Abstract

We consider a monolayer of graphene under uniaxial, tensile strain and simulate Bloch oscillations for different electric field orientations parallel to the plane of the monolayer using several values of the components of the uniform strain tensor, but keeping the Poisson ratio in the range of observable values. We analyze the trajectories of the charge carriers with different initial conditions using an artificial neural network, trained to classify the simulated signals according to the strain applied to the membrane. When the electric field is oriented either along the Zig-Zag or the Armchair edges, our approach successfully classifies the independent component of the uniform strain tensor with up to 90% of accuracy and an error of $\pm 1\%$ in the predicted value. For an arbitrary orientation of the field, the classification is made over the strain tensor component and the Poisson ratio simultaneously, obtaining up to 97% of accuracy with an error that goes from $\pm 5\%$ to $\pm 10\%$ in the strain tensor component and an error from $\pm 12.5\%$ to $\pm 25\%$ in the Poisson ratio.

Keywords: Bloch oscillations, Artificial neural networks, Strained graphene

1. Introduction

Modern material science has received a tremendous impact after the first isolation of graphene membranes [1], giving rise to the era of 2D materials. Graphene possesses a number of outstanding properties, ranging from tremendously high electric and thermal conductivities, transparency of the membranes and, on top of that, stiffness and flexibility [2, 3, 4, 5]. Thus, the manipulation of electric properties through mechanical means has given rise to the field of straintronics [6] in graphene and other materials (see [7] for a recent review). On theoretical grounds, mechanical deformations of graphene membranes are usually accounted for through a strain tensor that describes the deviation of the graphene curvature with respect to the ideal flat case. The effect is then seen in tilting and displacing of the Dirac points in reciprocal space plus a re-shaping of these points such that the isoenergetic contours of these cones is elliptical, namely, the Fermi velocity becomes anisotropic and of tensor nature [7].

Email addresses: `gonzalez@ifm.umich.mx` (J A González), `clopez@ifm.umich.mx` (C E López), `raya@ifm.umich.mx` (A Raya)