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# Landau levels in uniaxially strained graphene: A geometrical approach

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## HIGHLIGHTS

- The LLs in uniaxially strained graphene are found using a geometrical approach.
- The energy of the LLs in function of the Dirac cone deformation is presented.
- We found that uniaxial strain in graphene induces a contraction of the LLs spectra.
- Contraction in LLs spectra depends on the geometrical parameters of the Dirac cone.

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## ABSTRACT

The effect of strain on the Landau levels (LLs) spectra in graphene is studied, using an effective Dirac-like Hamiltonian which includes the distortion in the Dirac cones, anisotropy and spatial-dependence of the Fermi velocity induced by the lattice change through a renormalized linear momentum. We propose a geometrical approach to obtain the electron's wave-function and the LLs in graphene from the Sturm–Liouville theory, using the minimal substitution method. The coefficients of the renormalized linear momentum are fitted to the energy bands, which are obtained from a Density Functional Theory (DFT) calculation. In particular, we evaluate the case of Dirac cones with an ellipsoidal transversal section resulting from uniaxially strained graphene along the Arm-Chair (AC) and Zig-Zag (ZZ) directions. We found that uniaxial strain in graphene induces a contraction of the LLs spectra for both strain directions. Also, is evaluated the contribution of the tilting of Dirac

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cone axis resulting from the uniaxial deformations to the contraction of the LLs spectra.



## 1. Introduction

Graphene is a two-dimensional material conformed by hexagonal rings of carbon atoms with unique physical properties, which make it a material of great scientific and technological interest. Graphene shows an anomalous Hall effect at room temperature, resulting from a linear dependence between the density of electric charge carriers and the voltage [1–3]. An extraordinary feature of the electronic properties in graphene is the linear relation between energy and momentum of $2p_z$ electrons at low energies (less than 1 eV), being different than the usual quadratic energy momentum relations in ordinary materials. That dispersion relation ($E \propto k$) causes that the electron transport in graphene to be governed by a Dirac-like Hamiltonian, and electrons to behave like massless Dirac fermions [2–5]. The peculiar electronic properties of graphene have consequences on the Landau Levels (LLs) spectra, which are defined as quantized energy states of charged particles in motion under a uniform applied magnetic field, $B$ [6]. In an ordinary conductor, the energy of the LLs have a linear dependence with the quantization integer $n$, as $(n + 1/2)B$. However, in graphene the LLs spectrum is quantized according to $\sqrt{nB}$ [7–14].

In recent years, many works have been devoted to find practical methods to control graphene's properties. A possible way to modulate the electronic, vibrational and transport properties is by performing a deformation on the graphene sample [15–41] or bilayer graphene [42]. Thus, actual studies identify three main effects of uniaxial strain on low-energy band structure in graphene [15–20]. First, a slipping of the Dirac points out of the high symmetry points $K$ and $K'$. Second, a distortion in the traversal section of the Dirac cones, breaking the isotropy of the Fermi velocity; and third, a small vertical axis tilting of Dirac cones, which could be negligible in most of the situations. Considering that the LLs in graphene only depend on the shape of Dirac cone cross section, the second effect is expected to have more influence on the structure of LLs spectra. As we show here, the tilting of Dirac cone axis also has a non negligible effect on LLs for high strains (15%–20%).

Some theoretical works use an anisotropic mass model to find the LLs in graphene through topological considerations [14]. Other authors frequently analyze the properties of strained graphene using the Tight-Binding (TB) approximation, including the effect of deformation on the atomic distances through the scaling of the hopping parameters [13,15–19,21–29]. This hopping renormalization is commonly modeled with an exponential decay [43] or using Harrison's scaling rule $V_{pp\pi} \propto 1/l^2$ [44]. Both renormalizations could fail beyond the linear elastic regime since the Poisson ratio changes with the strain. Indeed they could have a different dependence for each strain-type considered. An accurate and precise way to obtain the hopping parameters in strained graphene is through a fitting of the TB Hamiltonian to the energy bands obtained from Density Functional Theory (DFT) calculations [30] or from experimental data.

Instead of a hopping renormalization, an alternative way is proposed in the present work. We use a renormalized linear momentum in an effective Dirac-like Hamiltonian. The coefficients of the linear momentum are related with the geometrical parameters of the distorted Dirac cone, and can be calculated from a fitting to the energy bands obtained with a DFT calculation. Then, we apply a minimal substitution in the free-field effective Dirac-like Hamiltonian to get the LLs spectra. In particular, for uniaxial strain we found that the LLs spectra are contracted as a function of the deformation along the Zig-Zag (ZZ) and Arm-Chair (AC) directions. This contraction of the LLs spectra is due to the renormalization of the Fermi velocity with the strain, which is reduced by the stretching along these directions. In addition, we have evaluated the contribution of the tilting of Dirac cone axis to the contraction of the LLs in uniaxially deformed graphene.