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EMANOEL MESSIAS DE LIMA BARBOSA

EFFECTS OF STRAIN IN $\alpha - T_3$ LATTICE AND ITS NANORIBBONS

FORTALEZA

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Dissertation submitted to the Programa de Pós-Graduação em Física of the Centro de Ciências of the Universidade Federal do Ceará, as a partial requirement for obtaining the title of Master in Physics. Concentration Area: Condensed Matter Physics

Advisor: Prof. Dr. Gil de Aquino Farias

Co-advisor: Prof. Dr. Diego Rabelo da Costa

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I dedicate it to my Mother, Maria da Conceição Gomes de Lima, who, behind the scenes, made everything happen!

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“Eu só queria que pelo menos um dos meus
filhos aprendesse a ler.”

(Maria da Conceição)

ABSTRACT

The $\alpha - T_3$ lattice, commonly regarded as a model system with a hexagonal structure containing an additional atom at the center of each hexagon, whose couplings to the surrounding sublattices are modulated by an intrinsic parameter α that continuously interpolates between the honeycomb lattice ($\alpha = 0$) and the dice lattice ($\alpha = 1$)—has attracted considerable interest within the condensed matter physics community owing to its unusual electronic and transport properties. Along this interpolation, the nature of the low-energy charge carriers in the $\alpha - T_3$ lattice evolves from spin- $S = 1/2$ Dirac fermions, as in graphene, to spin- $S = 1$ Dirac fermions characteristic of the dice lattice. Beyond the interpolation parameter α , additional mechanisms can be employed to tailor the physical properties of the $\alpha - T_3$ lattice, including geometric confinement in narrow nanoribbons, structural deformations of the lattice, and the application of external electric or magnetic fields. Motivated by this tunable morphological character and the associated quantum finite-size effects, this master’s thesis investigates how the electronic properties of the $\alpha - T_3$ lattice and its nanoribbons are modified under different types of uniform strain, specifically uniaxial, biaxial, and shear deformations. We systematically examine the influence of edge terminations (zigzag and armchair boundaries), the connectivity of the central atom in the hexagon to its neighboring sites, the ribbon width, and the magnitude and nature of the applied deformation. Our theoretical analysis, formulated in both first- and second-quantized forms, is based on a tight-binding Hamiltonian that captures, in the appropriate limits, the electronic structures of graphene and the dice lattice, including the coexistence of flat and conical bands. The resulting band structures reveal how the electronic properties evolve as functions of lattice morphology, orbital overlap, quantum confinement, and strain amplitude. We demonstrate that five out of the six considered types of in-plane uniform deformations (uniaxial strain, simple shear in the x and y directions, and pure shear) induce a finite energy gap in the band structure. Furthermore, we obtain analytical expressions that describe the monotonic increase of this gap with strain amplitude and its dependence on the underlying model parameters. For nanoribbons, we classify the systems as metallic or semiconducting and show how this classification can be altered by varying the lattice morphology, edge termination, and ribbon width. In addition, we demonstrate that the band gap can be effectively tuned by applying shear strain along the periodicity direction.

Keywords: electronic properties; tight-binding; $\alpha - T_3$ lattice; nanoribbons; strain.

RESUMO

A rede $\alpha - T_3$ — comumente considerada um sistema-modelo com estrutura hexagonal, contendo um átomo adicional no centro de cada hexágono, cujos acoplamentos às sub-redes circundantes são modulados por um parâmetro intrínseco α que interpola continuamente entre a rede em favo de mel ($\alpha = 0$) e a rede dice ($\alpha = 1$) — tem atraído considerável interesse na comunidade de física da matéria condensada devido às suas propriedades eletrônicas e de transporte incomuns. Ao longo dessa interpolação, a natureza dos portadores de carga de baixa energia na rede $\alpha - T_3$ evolui de férmions de Dirac com spin $S = 1/2$, como no grafeno, para férmions de Dirac com spin $S = 1$, característicos da rede *dice*. Para além do parâmetro de interpolação α , mecanismos adicionais podem ser empregados para ajustar as propriedades físicas da rede $\alpha - T_3$, incluindo confinamento geométrico em nanofitas estreitas, deformações estruturais da rede e a aplicação de campos elétricos ou magnéticos externos. Motivada por esse caráter morfológico ajustável e pelos correspondentes efeitos quânticos de tamanho finito, esta dissertação de mestrado investiga como as propriedades eletrônicas da rede $\alpha - T_3$ e de suas nanofitas são modificadas sob diferentes tipos de deformações uniformes, em particular deformações uniaxiais, biaxiais e de cisalhamento. Examinamos sistematicamente a influência das terminações de borda (contornos zigzag e armchair), da conectividade do átomo central do hexágono com seus sítios vizinhos, da largura da fita e da magnitude e da natureza da deformação aplicada. Nossa análise teórica, formulada tanto em primeira quanto em segunda quantização, baseia-se em um hamiltoniano de tight-binding que reproduz, nos limites apropriados, as estruturas eletrônicas do grafeno e da rede dice, incluindo a coexistência de bandas planas e cônicas. As estruturas de bandas resultantes revelam como as propriedades eletrônicas evoluem em função da morfologia da rede, do recobrimento orbital, do confinamento quântico e da amplitude de deformação. Demonstramos que cinco dos seis tipos de deformações uniformes no plano considerados (deformação uniaxial, cisalhamento simples nas direções x e y e cisalhamento puro) induzem a abertura de um gap de energia finito na estrutura de bandas. Além disso, obtemos expressões analíticas que descrevem o aumento monótono desse *gap* em função da amplitude de deformação e de sua dependência dos parâmetros do modelo. Para nanofitas, classificamos os sistemas como metálicos ou semicondutores e mostramos como essa classificação pode ser alterada ao variar a morfologia da rede, a terminação de borda e a largura da fita. Adicionalmente, demonstramos que o gap de

banda pode ser ajustado eficientemente aplicando uma deformação de cisalhamento na direção de periodicidade.

Keywords: propriedades eletrônicas; *tight-binding*; rede $\alpha - T_3$; nanofitas; deformação.

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LIST OF ABBREVIATIONS AND ACRONYMS

$A\alpha - T_3\text{NRs}$	Armchair $\alpha - T_3$ nanoribbons
DOS	Density of states
HCL	Honeycomb Lattice
LCAO	Linear Combinations of Atomic Orbitals
TB	Tight-Binding Method
$Z\alpha - T_3\text{NRs}$	Zigzag $\alpha - T_3$ nanoribbons

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1 INTRODUCTION

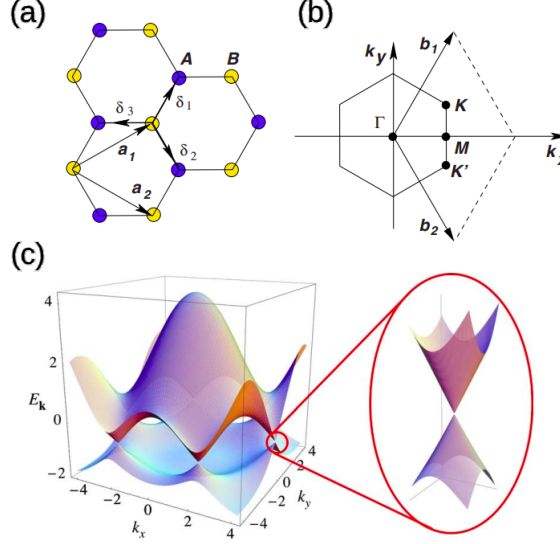
1.1 2D Materials beyond graphene with flat bands

The isolation of graphene in mid-2004 via micromechanical exfoliation stimulated intense interest in novel two-dimensional (2D) materials exhibiting comparable electronic and/or mechanical properties, particularly because their electronic characteristics are potentially suitable for the realization of electronic devices (NETO *et al.*, 2009). In graphene, the charge carriers display zero-gap semiconductor behavior: the valence and conduction bands touch at the corners of the first Brillouin zone, at the so-called K and K' Dirac points (see Fig. 1). To induce a finite bandgap and thereby control the carrier character (metallic versus semiconducting), several graphene-based system architectures have been proposed, including multilayers, nanoribbons, chemical doping, external electric and magnetic fields, and mechanical deformation, among others (SENA *et al.*, 2012).

From a broader perspective on 2D materials, the last two decades have witnessed substantial advances in this field, emphasizing properties of particular interest, notably electronic properties, which are strongly correlated with the underlying atomic geometry (SLOT *et al.*, 2017). Consequently, an inverse design paradigm has emerged: rather than first synthesizing 2D materials and subsequently characterizing their electronic properties, numerous theoretically designed materials with prescribed geometries are proposed, and their key features are investigated computationally and discussed in the literature. Only after this theoretical screening is the experimental synthesis of the most promising 2D systems pursued.

Certain specific lattice geometries give rise to unconventional electronic band structures, such as conical (Dirac-like) and flat bands. Materials exhibiting conical bands with vanishing bandgap possess several remarkable features, particularly in the low-energy regime, where electrons behave as massless fermionic quasiparticles. This arises because the energy-momentum dispersion can, in this case, be approximated as a linear function of momentum, which in turn is described by the Dirac equation (MALKO *et al.*, 2012). Such systems are referred to as 2D Dirac materials, and their hallmark physical properties include the half-integer quantum Hall effect, enhanced carrier mobility, and Klein tunneling (LIU *et al.*, 2023; ALLAIN; FUCHS, 2011).

Figure 1 – Schematic representation of the crystalline lattice of graphene (a). Panel (b) shows the corresponding first Brillouin zone, while panel (c) depicts the electronic band structure, including a magnified view of the region where the valence and conduction bands touch.

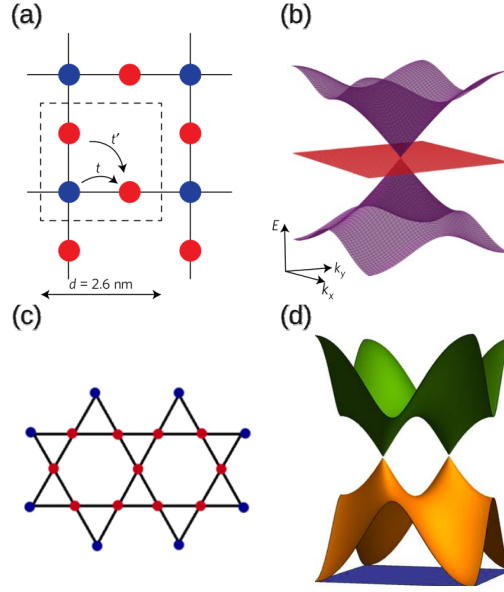


Source: Figure adapted from reference (NETO *et al.*, 2009).

Materials exhibiting flat electronic bands display a broad range of nontrivial physical phenomena, including super-Klein tunneling, high-temperature ferromagnetism, and superconductivity (ILLES; NICOL, 2017b; UCHOA, 2023). In such systems, the electronic structure is characterized by a large density of states associated with vanishing kinetic energy. Another salient feature is the unconventional charge transport, arising from the nearly zero group velocity of the flat-band states in the vicinity of the Fermi level (DEPENBROCK *et al.*, 2012).

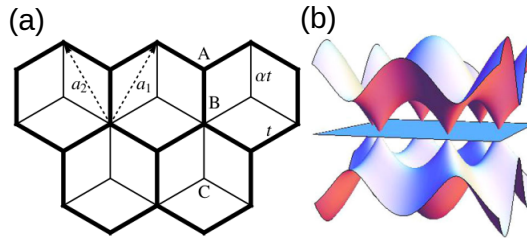
From a theoretical standpoint, the $\alpha - T_3$ model and the Lieb lattice represent minimal tight-binding models that exhibit flat-band characteristics in their energy spectra. Additionally, the Kagome lattice constitutes another paradigmatic example of a system hosting flat bands. Figures 2 and 3 schematically depict the Lieb, Kagome, and $\alpha - T_3$ lattices, respectively, together with their corresponding band dispersion relations.

Figure 2 – Illustration of the crystal structure of the (a) Lieb and (c) Kagome lattices and their band structures in (b) and (d), respectively.



Source: Figure adapted from references (SLOT *et al.*, 2017; LIM *et al.*, 2020).

Figure 3 – (a) Sketch of the crystal structure of the $\alpha - T_3$ lattice and (b) its respective band structure.



Source: Figure adapted from reference (RAOUX *et al.*, 2014).

As shown in Figs. 2 and 3, the energy spectra of the Lieb and $\alpha - T_3$ lattices are characterized by a three-band structure in which a flat band intersects the Dirac points at which the conduction and valence bands meet. The spectra of these lattices exhibit electron–hole symmetry, analogous to the case of graphene (LIN *et al.*, 2023). These systems have attracted considerable attention because their low-energy excitations can be effectively described by an enlarged pseudospin $S = 1$ formalism (BETANCUR-OCAMPO *et al.*, 2017).

Within the broader class of flat-band materials, we focus specifically on the $\alpha - T_3$ lattice, which constitutes the central subject of this dissertation. The $\alpha - T_3$ model

was originally proposed in the context of ultracold atoms in optical lattices in a 2014 study (RAOUX *et al.*, 2014), where it was shown to exhibit a transition in the orbital magnetic response from diamagnetic ($\alpha = 0$) to paramagnetic ($\alpha = 1$). This transition has recently been associated with the evolution of the Berry phase in this system, which varies continuously from π to 0 as the lattice is tuned from the honeycomb to the dice limit, respectively (ILLES, 2017). Structurally, the $\alpha - T_3$ lattice is a theoretical two-dimensional (2D) material with a hexagonal geometry similar to graphene, but with an additional atomic site located at the center of each hexagon. The nearest-neighbor hopping amplitude t between the corner sites of the hexagon (atoms A and B) and the central site (atom C) is modulated by a tunable parameter $0 \leq \alpha \leq 1$, enabling a continuous interpolation between graphene ($\alpha = 0$) and the dice lattice ($\alpha = 1$).

This structural peculiarity, which permits a continuous interpolation between the graphene ($\alpha = 0$) and dice ($\alpha = 1$) limits, is particularly noteworthy, as both endpoint systems have been extensively investigated from theoretical and experimental perspectives. Moreover, it has recently been shown that a 2D model for $Hg_{1-x}Cd_xTe$ at critical doping can be mapped onto an $\alpha - T_3$ model with an intermediate parameter value $\alpha = 1/\sqrt{3}$ (MALCOLM; NICOL, 2015). From an experimental standpoint, the realization of a pseudospin-1 dice lattice has been proposed via the growth of a trilayer structure of cubic perovskites, such as $SrTiO_3/SrIrO_3/SrTiO_3$ along the (111) direction, or by trapping ultracold atoms in suitably engineered optical lattices (WANG *et al.*, 2020; WANG; RAN, 2011). These developments underscore the importance of studying interpolating models, such as the $\alpha - T_3$ lattice, for understanding emergent phenomena in flat-band systems.

1.2 2D Materials Nanoribbons

Nanoribbons of 2D materials are defined so as to preserve the underlying lattice geometry and its translational periodicity along one spatial direction, while being laterally confined in the transverse direction to a width on the nanometric scale. Research on nanoribbons is of central importance in the search for novel nanoscale devices, since their physical properties can be systematically tailored by multiple means, including chemical doping, introduction of defects, mechanical deformation, width modulation, control of edge morphology, and the application of external electric and magnetic fields (SHINDE *et al.*, 2022).

The term “morphology” in this context refers to the detailed shape of the nanoribbon edges and to its width, typically quantified by the number of atomic rows across the transverse direction. These morphological characteristics give rise to several distinctive features, such as the emergence of metallic or semiconducting behavior in specific materials (CHANG *et al.*, 2007). The possible edge terminations of a given nanoribbon depend on the crystal structure of the parent 2D material. For instance, graphene nanoribbons most commonly exhibit zigzag and armchair edge terminations, whereas Lieb-lattice nanoribbons display straight, barbed, and asymmetric edges, and Kagome-lattice nanoribbons are known to host zigzag and sawtooth terminations.

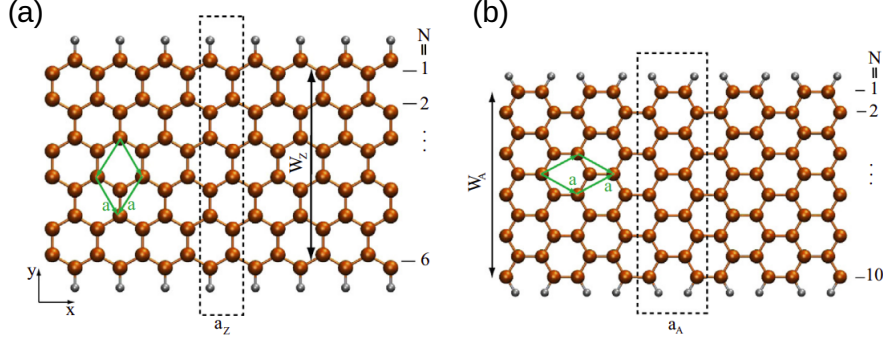
Within this framework, we investigate graphene and $\alpha - T_3$ nanoribbons, each realized with both zigzag and armchair edge terminations. We analyze their response to mechanical deformation and investigate the systematic dependence of their electronic band structures on ribbon width.

1.2.1 Graphene Nanoribbons

As observed, the band structure of bulk graphene (see Fig. 1(c)) exhibits no energy gap: the valence and conduction bands touch at the Dirac points, rendering the system intrinsically metallic. In this context, graphene nanoribbons emerge as a strategy to circumvent this limitation, since the quantum confinement of the electronic wave functions, together with edge effects, induces the opening of a band gap that can be tuned by varying the nanoribbon width (TABARRAEI *et al.*, 2015).

We now focus on the crystallographic properties of graphene nanoribbons. As previously discussed, the most common edge terminations are the zigzag and armchair types (see Fig. 4). In both cases, the ribbon width W is directly related to the number of atomic lines across the transverse direction.

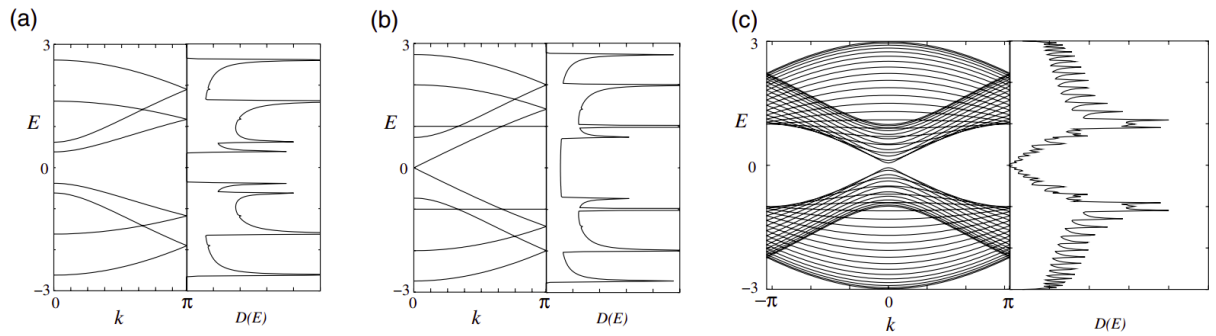
Figure 4 – Crystallographic structure of graphene nanoribbons with zigzag and armchair edge terminations. The green parallelogram with edge length a represents the unit cell of bulk graphene, while the dashed rectangles indicate the unit cells of the corresponding nanoribbons.



Source: Figure adapted from reference (TABARRAEI *et al.*, 2015).

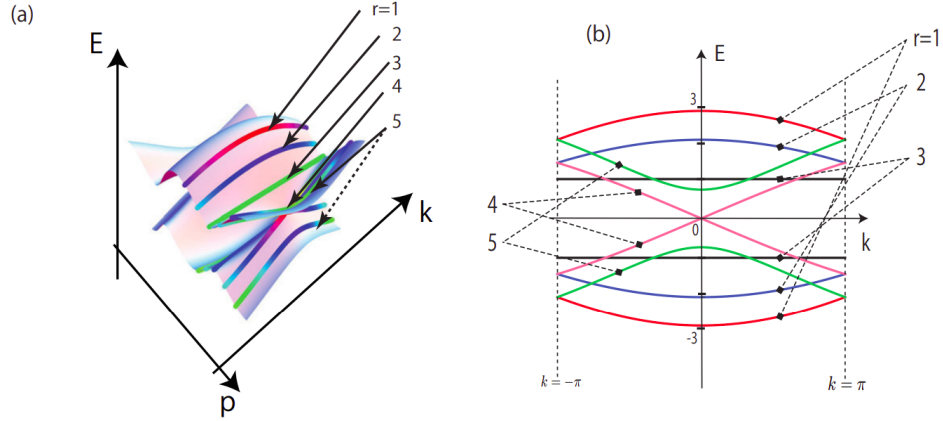
The band dispersion of armchair graphene nanoribbons is strongly dependent on their width, as shown in Fig. 5. Theoretical studies indicate that armchair-terminated nanoribbons are semiconducting for widths W corresponding to atomic line numbers $N = 3m$ and $N = 3m + 1$ (with m a positive integer), and metallic for $N = 3m + 2$. Another important feature is that, as N increases, the energy spectrum progressively approaches that of the infinite graphene lattice (bulk limit). This convergence is illustrated in Fig. 6, which shows the energetic projection of the nanoribbon dispersion relation onto the bulk band structure.

Figure 5 – Band structures $E(k)$ and densities of states $D(E)$ of armchair graphene nanoribbons for different numbers of atomic lines N : (a) $N = 4$, (b) $N = 5$, and (c) $N = 30$.



Source: Figure adapted from reference (WAKABAYASHI *et al.*, 2010).

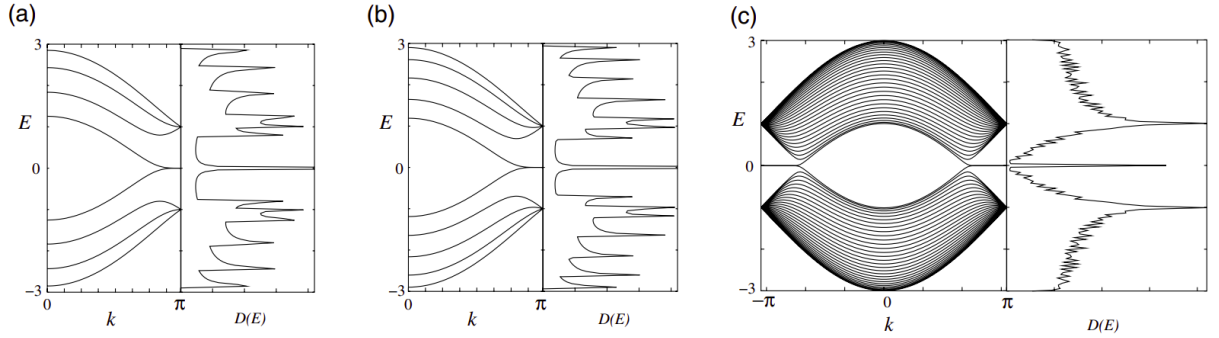
Figure 6 – Energetic projection of the dispersion relation of an armchair graphene nanoribbon with $N = 5$ atomic lines onto the bulk band structure.



Source: Figure adapted from reference (WAKABAYASHI *et al.*, 2010).

In contrast, for zigzag edge terminations, the metallic or semimetallic character is not governed by the number of atomic lines. Instead, it arises from the degeneracy of the valence and conduction bands at $k = \pi$, as shown in the dispersion relation in Fig. 7.

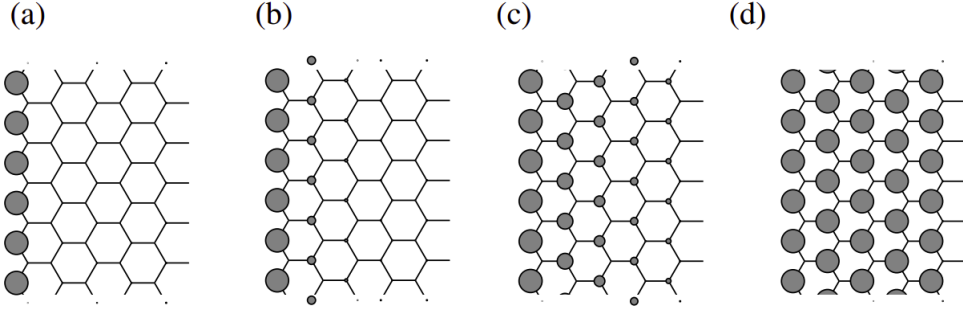
Figure 7 – Band structures $E(k)$ and densities of states $D(E)$ of zigzag graphene nanoribbons for different numbers of atomic lines N : (a) $N = 4$, (b) $N = 5$, and (c) $N = 30$.



Source: Figure adapted from reference (WAKABAYASHI *et al.*, 2010).

The spatial distribution of the electronic states in the vicinity of the Fermi level for different values of the wave vector k is illustrated in Figs. 8(a)–8(d). In these figures, the radius of each sphere is proportional to the local probability density. In particular, for $k = \pi$, the electronic density is strongly localized at the ribbon edges, giving rise to the so-called edge states. This feature is characteristic of systems with zigzag edge terminations. For values of k away from this point, the probability density is distributed throughout the interior of the nanoribbon.

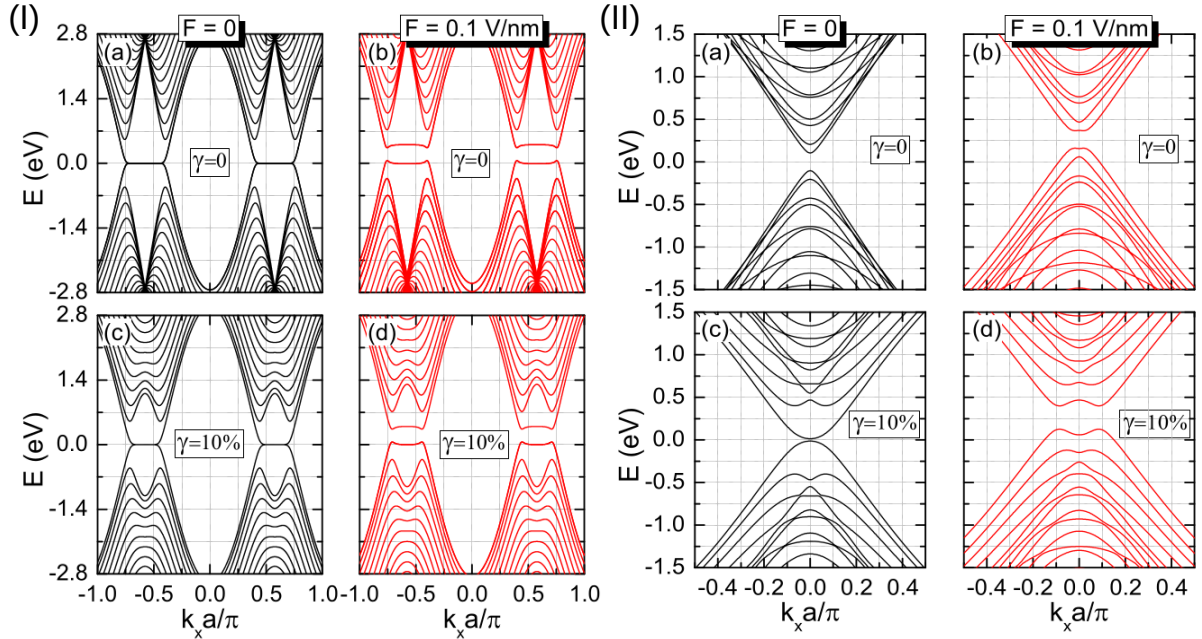
Figure 8 – Probability density of edge states for different values of the wave vector k : (a) $k = \pi$, (b) $k = 8\pi/9$, (c) $k = 7\pi/9$, and (d) $k = 2\pi/3$. The radius of the spheres is proportional to the corresponding probability density.



Source: Figure adapted from reference (WAKABAYASHI *et al.*, 2010).

The application of an external electric field and simple-shear strain are mechanisms capable of modifying the electronic band structure (BANDEIRA *et al.*, 2020). Figure 9 illustrates the response of the band structure of graphene nanoribbons to the application of an in-plane electric field and simple shear stress along the periodic direction.

Figure 9 – Band structure of graphene nanoribbons under an applied electric field, denoted by F , and shear strain, denoted by γ , for zigzag and armchair edge terminations, respectively.



Source: Figure adapted from reference (BANDEIRA *et al.*, 2020).

For the zigzag termination, the application of the electric field induces the opening of a small energy gap, which is preserved under the combined application of electric field and shear strain, as shown in Figs. 9(I b and d). In the case of the (nominally

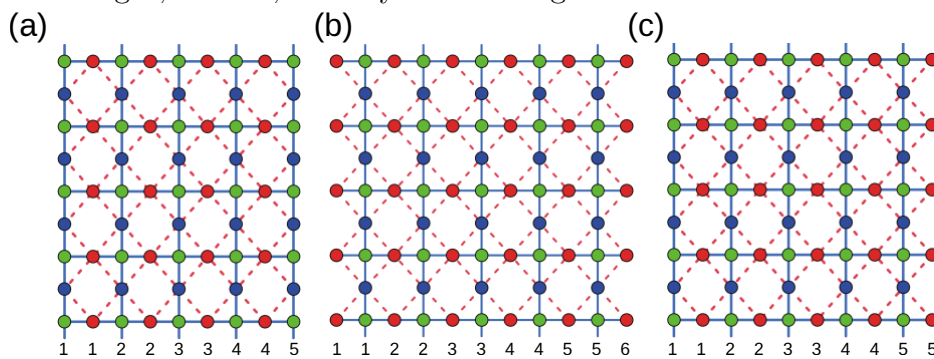
metallic) armchair termination, the application of simple shear closes the pre-existing energy gap, whereas the simultaneous application of electric field and shear reopens the gap, see Figs. 9(II c and d).

In summary, graphene nanoribbons may exhibit either metallic or semiconducting behavior, depending on their width and edge termination. However, morphology is not the only factor that can modulate their electronic properties. As demonstrated for both edge terminations, the combined application of an in-plane electric field and simple shear along the periodic direction results in the opening of an energy gap in both types of graphene nanoribbon edges.

1.2.2 Lieb Nanoribbons

The Lieb lattice, similarly to the $\alpha - T_3$ lattice, exhibits a flat band in its energy spectrum, as shown in Fig. 2(b). Its band structure consists of three bands with electron-hole symmetry, in which a flat band touches two linearly dispersing bands at a single Dirac point (CHEN; ZHOU, 2016). Lieb nanoribbons can present three distinct types of edge termination—straight, barbed, and asymmetric—as illustrated in Fig. 10.

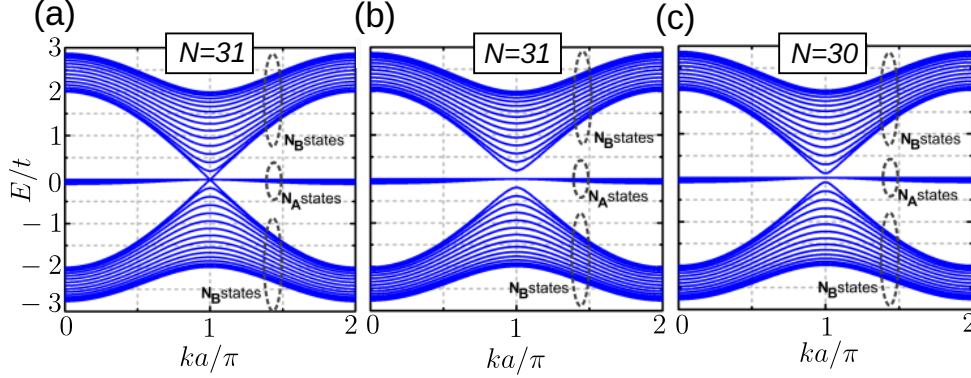
Figure 10 – (Color online) Crystallographic structure of Lieb lattice nanoribbons with straight, barbed, and asymmetric edge terminations.



Source: Figure adapted from reference (CHEN; ZHOU, 2016).

The corresponding energy band structures for these different edge terminations are shown below. An energy gap is observed only for nanoribbons with barbed and asymmetric edges, with the latter exhibiting a smaller gap.

Figure 11 – Band structure of Lieb lattice nanoribbons with straight, barbed, and asymmetric edge terminations, respectively. N_A , N_B , and N_C denote the numbers of atomic rows in the nanoribbon associated with sites A, B, and C.



Source: Figure adapted from reference (UCHOA, 2023).

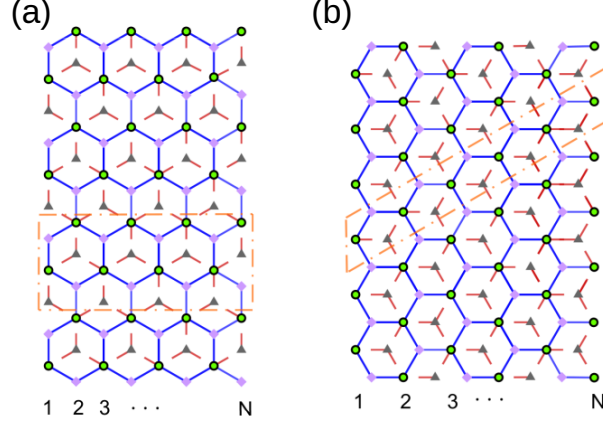
1.2.3 $\alpha - T_3$ Nanoribbons

The $\alpha - T_3$ lattice is a theoretical 2D material characterized by a hexagonal structure analogous to that of graphene, but with an additional atom placed at the center of each hexagon. The nearest-neighbor hopping interaction t between the atoms located at the vertices of the hexagon (sublattices A and B) and the central atom (sublattice C) is modulated by a tunable parameter $0 \leq \alpha \leq 1$. This parameter enables a continuous interpolation between the graphene lattice ($\alpha = 0$), in which the central site is completely decoupled, and the dice lattice ($\alpha = 1$), where the coupling to the central site is maximal (RAOUX *et al.*, 2014).

As in graphene, $\alpha - T_3$ nanoribbons may exhibit zigzag or armchair edge terminations, as illustrated in Fig. 12. Owing to the presence of three inequivalent atoms in the unit cell, the zigzag termination can occur in three distinct configurations: zigzag A–A, zigzag A–B, and zigzag A–C. In contrast, armchair terminations necessarily expose all three atomic species at the edges. A salient feature of this material is the presence of a flat, non-dispersive energy band in its electronic spectrum, as shown in Fig. 3. Recent work by Li *et al.* (2022) has demonstrated that the application of an external electric field (along the finite-width direction of the ribbon) and a perpendicular magnetic field to $\alpha - T_3$ nanoribbons substantially modifies their band structure, including the originally non-dispersive flat band, as illustrated in Fig. 13.

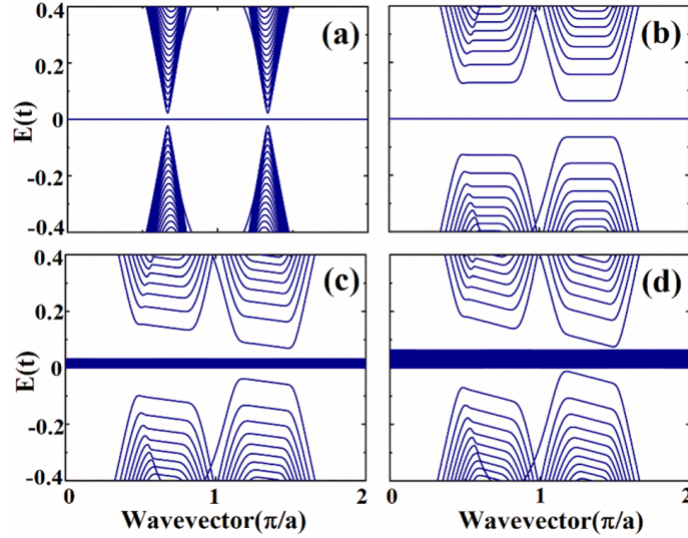
The system under consideration exhibits a finite energy gap between the valence and conduction bands, and therefore behaves as a semiconductor. The application of a

Figure 12 – (Color online) Crystallographic structure of the $\alpha - T_3$ nanoribbon with armchair- and zigzag-type edge terminations. The dotted-dashed rectangle and parallelogram indicate the unit cell of the nanoribbons.



Source: Figure adapted from reference (CHEN *et al.*, 2019).

Figure 13 – (Color online) Band structure of an $\alpha - T_3$ nanoribbon with A-C zigzag edge termination for $\alpha = 0.5$ under different values of magnetic flux ϕ and transverse electric field eE_y . (a) $\phi = 0$ and $eE_y = 0$. (b) $\phi = 0.0015$ and $eE_y = 0$. (c) $\phi = 0.0015$ and $eE_y = 0.001$ t/nm. (d) $\phi = 0.0015$ and $eE_y = 0.002$ t/nm.



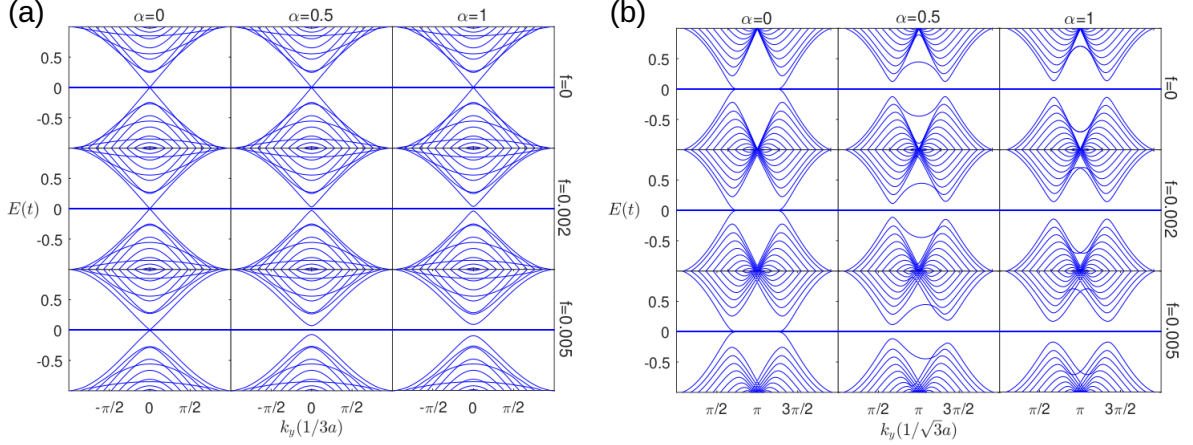
Source: Figure adapted from Ref. (LI *et al.*, 2022).

perpendicular magnetic field modifies the band structure in a valley-asymmetric manner, *i.e.*, the two inequivalent valleys are distorted differently. Consequently, the magnetic field induces a valley polarization of the spectrum, as shown in Fig. 13(b). In addition, the band gap increases in the presence of the magnetic field. The simultaneous application of electric and magnetic fields produces a combined effect: the valley polarization is maintained, while the originally flat (non-dispersive) band becomes discretized and splits into multiple dispersive subbands whose number and dispersion increase with the electric field strength,

as illustrated in Figs. 13(c) and 13(d).

As previously discussed, the $\alpha - T_3$ lattice provides a continuous interpolation between graphene ($\alpha = 0$) and the dice lattice ($\alpha = 1$). Below, we present the corresponding band structures for selected values of the parameter α .

Figure 14 – Band structure of $\alpha - T_3$ nanoribbons with armchair and A–C zigzag edge terminations for $\alpha = 0, 0.5, 1$ and different magnetic flux values $\phi = 0, 0.002, 0.005$. The ribbon width is fixed at $N = 20$.



Source: Figure adapted from Ref. (CHEN *et al.*, 2019).

For nanoribbons with armchair edge termination, the band structure is only weakly dependent on the parameter α . In this geometry, the magnetic field opens a small band gap, which increases as the magnetic flux is enhanced, as can be observed in Fig. 14(a). In contrast, nanoribbons with zigzag edge termination exhibit a pronounced sensitivity to variations in α as well as to the magnetic field, as evidenced in Fig. 14(b).

In summary, $\alpha - T_3$ nanoribbons can display either metallic or semiconducting behavior depending on intrinsic parameters, such as α , and extrinsic control parameters, such as an applied magnetic field. For intermediate values of α (e.g., away from the graphene and dice limits), the magnetic field induces a significant polarization of the spectrum in zigzag nanoribbons. The electric field predominantly affects the flat band, rendering it dispersive and leading to its transformation into a set of dispersive subbands.

1.3 Scope of dissertation

Motivated by the morphological features of the $\alpha - T_3$ lattice and by quantum size and external-field effects, we use a tight-binding model to study how its electronic properties and those of its nanoribbons depend on intrinsic parameters—edge terminations

(zigzag and armchair), connections between the central atom and its neighbors, ribbon width—and on extrinsic parameters such as strain.

In Chapter 2, we examine the crystallography of the $\alpha - T_3$ lattice, introduce the tight-binding model in first and second quantization, and describe its electronic properties in both formalisms. We then analyze a continuum model to describe electron behavior via a Dirac-like equation.

In Chapter 3, we apply the tight-binding model in second quantization and the Heisenberg equation of motion to $\alpha - T_3$ nanoribbons, investigating how their electronic properties depend on edge termination, ribbon width, and related morphological details, including limiting and transition cases.

In Chapter 4, we incorporate uniform strain fields into the tight-binding model to study their effects on the electronic properties of the $\alpha - T_3$ lattice. After introducing elasticity theory and the description of deformations in real and reciprocal space for 2D materials, we analyze six types of planar strain in the infinite lattice: uniaxial (along x and y), biaxial, simple shear (along x and y), and pure shear. We then apply simple shear strain to $\alpha - T_3$ nanoribbons with both edge terminations.

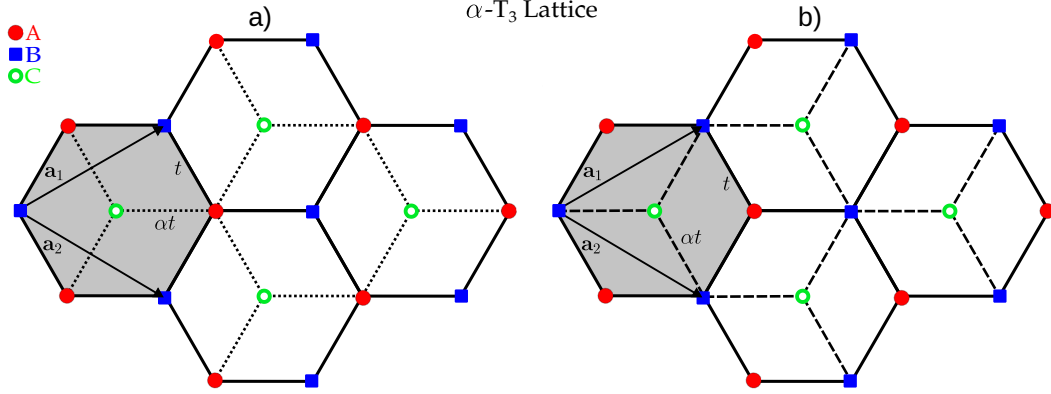
In Chapter 5, we summarize the main conclusions and highlight results, and discuss perspectives for future work.

2 TIGHT-BINDING HAMILTONIAN OF $\alpha - T_3$ MODEL FIRST AND SECOND QUANTIZATION APPROACH

2.1 Crystallographic Aspects of $\alpha - T_3$ Lattice

The discovery of graphene has significantly intensified the search for novel 2D materials. Consequently, a wide variety of theoretically proposed systems with analogous electronic characteristics has emerged, among which the $\alpha - T_3$ lattice is a prominent example. The $\alpha - T_3$ lattice is a crystalline structure whose unit cell contains three inequivalent sites, denoted A , B , and C . The central site C is coupled to the surrounding sites through a tunable hopping amplitude αt (ILLES, 2017), as illustrated in Fig. 15.

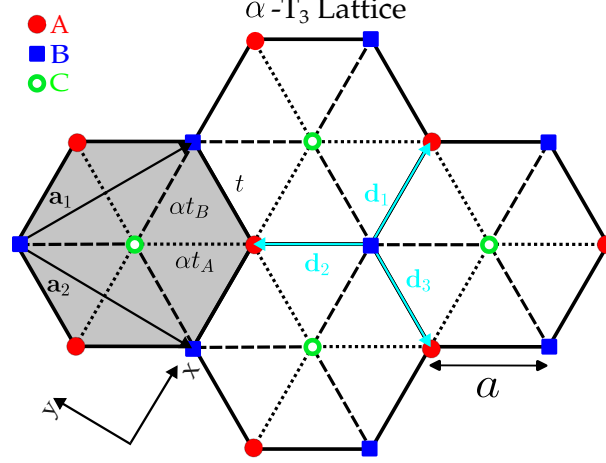
Figure 15 – The $\alpha - T_3$ lattice with two types of connections between the A (red circle), B (blue square) and C (green circle) sites. In gray, we have the unit cell.



Source: The author.

The variable parameter α ranges from 0 to 1, where $\alpha = 0$ corresponds to a graphene-like model and $\alpha = 1$ corresponds to the dice lattice. Figure 15 depicts two variants of the $\alpha - T_3$ lattice that are frequently discussed in the literature, typically only one at a time. Nonetheless, when this model was originally introduced, the possibility of its extension to encompass such variants was already noted (PIÉCHON *et al.*, 2015). In order to incorporate both configurations and systematically analyze their properties, we introduce the theoretical model shown in Fig. 16, which simultaneously accounts for both lattice formats. By considering the hopping parameters as either $t_A = t$, $t_B = 0$ or $t_A = 0$, $t_B = t$, we recover, respectively, configurations (a) and (b) of Fig. 15.

Figure 16 – The $\alpha - T_3$ lattice model depicting two distinct types of couplings between the HCL and the central site C . The coupling amplitude t_A is indicated by dotted lines, whereas the coupling amplitude t_B is represented by dashed lines. The gray region denotes the unit cell, which consists of three inequivalent lattice sites, labeled A , B , and C .



Source: The author.

We now proceed to analyze the crystallographic properties of the $\alpha - T_3$ lattice. As shown in Fig. 16, the primitive lattice vectors $\mathbf{a}_1$ and $\mathbf{a}_2$, which connect the inequivalent lattice sites, are given by

$$\mathbf{a}_1 = \frac{3a}{2} \hat{x} + \frac{\sqrt{3}a}{2} \hat{y}, \quad (2.1)$$

and

$$\mathbf{a}_2 = \frac{3a}{2} \hat{x} - \frac{\sqrt{3}a}{2} \hat{y}. \quad (2.2)$$

where a denotes the lattice spacing, i.e., the distance between nearest-neighbor (NN) sites. From Eqs. (2.1) and (2.2), the corresponding reciprocal lattice vectors can be obtained using

$$\mathbf{b}_i = 2\pi \frac{\mathbf{a}_j \times \mathbf{a}_k}{\mathbf{a}_i \cdot (\mathbf{a}_j \times \mathbf{a}_k)}, \quad (2.3)$$

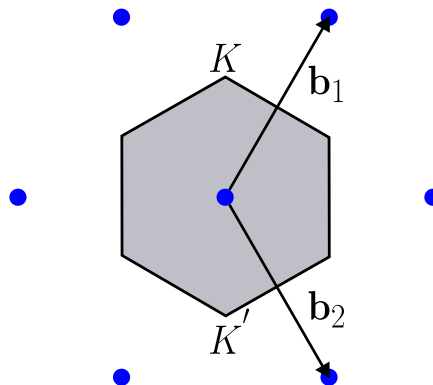
which yields

$$\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)} = \frac{2\pi}{3a} \hat{x} + \frac{2\pi\sqrt{3}}{3a} \hat{y}, \quad (2.4)$$

$$\mathbf{b}_2 = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)} = \frac{2\pi}{3a} \hat{x} - \frac{2\pi\sqrt{3}}{3a} \hat{y}, \quad (2.5)$$

where $\mathbf{a}_3 = (0, 0, 1)$. The resulting first Brillouin zone of this two-dimensional lattice is a regular hexagon, as illustrated schematically below.

Figure 17 – The reciprocal lattice vectors of the $\alpha - T_3$ model showing the hexagonal Brillouin zone, the reciprocal lattice vectors $\mathbf{b}_1$ and $\mathbf{b}_2$ and the K and K' points which are given, respectively, by $(0, \frac{4\pi}{3\sqrt{3}a})$ and $(0, -\frac{4\pi}{3\sqrt{3}a})$.



Source: The author.

Having established the geometric model and the crystallographic characterization of the $\alpha - T_3$ lattice, we now proceed to employ the Tight-Binding Method (TB) model to analyze its electronic properties. To this end, the methodological details will be presented in the subsequent sections.

2.2 The Tight-Binding Model for $\alpha - T_3$ Lattice in the First Quantization

The TB method, originally proposed by Bloch in 1928, is based on expanding the crystalline eigenstates in terms of a Linear Combinations of Atomic Orbitals (LCAO) constructed from the atomic orbitals of the constituent atoms (GROSSO; PARRAVICINI, 2013; LIMA *et al.*, 2022; DRESSELHAUS *et al.*, 2018). The central postulate is that, given the solutions of the Schrödinger equation for an isolated atom, these solutions can be used as an approximate basis that also satisfies the Schrödinger equation when the atoms are assembled to form a crystalline solid. This approach is particularly suitable for describing electrons occupying inner atomic shells, which retain a relatively localized character in the solid state. Conversely, this assumption breaks down for delocalized valence electrons in metals; for such electrons, a weak-binding (nearly-free-electron) approximation provides a more appropriate description (DRESSELHAUS *et al.*, 2018). The model can be applied to a wide range of systems, including molecules, polymers, nanotubes, and 2D and 3D crystals, and to calculations of the energy spectrum for 2D systems with one, two, and three energy bands (LIMA *et al.*, 2022). Given these general assumptions of the method, we will describe how to.

The TB formalism in first quantization is defined in terms of the Bloch functions, which are expressed as

$$\Phi_j(\mathbf{r}, \mathbf{k}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}_i} e^{i\mathbf{k} \cdot \mathbf{R}_i} \phi_j(\mathbf{r} - \mathbf{R}_i), \quad (2.6)$$

where $\mathbf{R}_i$ denotes the position of the i -th atomic site hosting the corresponding localized orbital $\phi_j(\mathbf{r} - \mathbf{R}_i)$, N is the total number of unit cells in the crystal, and $\mathbf{k}$ is a wave vector in the reciprocal lattice. Equation (2.6) satisfies Bloch's theorem, which characterizes the structure of wave functions in a periodic potential, here specifically the periodic potential of the crystalline solid¹. Within the tight-binding (TB) approximation, the electronic energy bands of a crystalline solid are obtained by solving a generalized eigenvalue problem.

$$\det||H_{jj'} - ES_{jj'}|| = 0. \quad (2.7)$$

The elements $H_{jj'}$ and $S_{jj'}$ constitute, respectively, the elements of the transfer integral matrix and the overlap matrix. These matrices are expressed in terms of the block function defined in Eq. (2.6) as follows:

$$H_{jj'} = \langle \Phi_j | H | \Phi_{j'} \rangle = \frac{1}{N} \sum_{\mathbf{R}'_i, \mathbf{R}_i} e^{i\mathbf{k} \cdot (\mathbf{R}'_i - \mathbf{R}_i)} t_{\mathbf{R}'_i, \mathbf{R}_i}^{jj'}, \quad (2.8)$$

$$S_{jj'} = \langle \Phi_j | \Phi_{j'} \rangle = \frac{1}{N} \sum_{\mathbf{R}'_i, \mathbf{R}_i} e^{i\mathbf{k} \cdot (\mathbf{R}'_i - \mathbf{R}_i)} s_{\mathbf{R}'_i, \mathbf{R}_i}^{jj'}, \quad (2.9)$$

where $t_{\mathbf{R}'_i, \mathbf{R}_i}^{jj'} = \langle \phi_j(\mathbf{r} - \mathbf{R}_i) | H | \phi_{j'}(\mathbf{r} - \mathbf{R}'_i) \rangle$ and $s_{\mathbf{R}'_i, \mathbf{R}_i}^{jj'} = \langle \phi_j(\mathbf{r} - \mathbf{R}_i) | \phi_{j'}(\mathbf{r} - \mathbf{R}'_i) \rangle$ denote, respectively, the hopping and overlap parameters. These quantities are more fundamental in nature and are typically obtained from first-principles calculations (DRESSELHAUS *et al.*, 2018).

The hopping parameter (or transfer integral) characterizes the energy associated with the electronic “hopping” process between lattice sites. More specifically, this term is related to the energy required for an electron to move from a site at position $\mathbf{R}'$ to a site at position $\mathbf{R}$, or vice versa (LIMA *et al.*, 2022). In contrast, the overlap parameter quantifies the spatial overlap between the atomic orbitals centered at the sites $\mathbf{R}'$ and $\mathbf{R}$. For well-localized atomic orbitals, the overlap between atomic-like functions centered on distinct lattice sites is typically small.

¹ For a more detailed treatment of the topic, see Refs. (DRESSELHAUS *et al.*, 2018; GROSSO; PARRAVICINI, 2013; KITTEL; MCEUN, 2018).

In the limiting case where the localized atomic orbitals are assumed to form an orthonormal set, the overlap matrix reduces to the identity matrix; that is, all off-diagonal elements vanish, while the diagonal elements are equal to unity. We now apply the procedure described above to determine the energy band structure of the $\alpha - T_3$ lattice.

As discussed in the section on crystallographic properties, the $\alpha - T_3$ lattice is a crystal structure whose unit cell contains three inequivalent sites, denoted A , B , and C . Consequently, the electronic energy dispersion relations are obtained by solving the eigenvalue problem for a 3×3 Hamiltonian matrix H and a 3×3 overlap matrix S associated with these three nonequivalent atomic orbitals. The Bloch orbitals constructed from the atomic orbitals on the A , B , and C sites can be written as

$$\Phi_j(\mathbf{r}, \mathbf{k}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}_i} e^{i\mathbf{k} \cdot \mathbf{R}_i} \phi_j(\mathbf{r} - \mathbf{R}_i), \quad j = \{A, B, C\}, \quad (2.10)$$

where N is the total number of unit cells and $\mathbf{R}_i$ denotes the lattice vectors.

The Hamiltonian and overlap matrices defined in Eqs. (2.8) and (2.9) for the $\alpha - T_3$ lattice thus take the form

$$H = \begin{pmatrix} H_{AA} & H_{AB} & H_{AC} \\ H_{BA} & H_{BB} & H_{BC} \\ H_{CA} & H_{CB} & H_{CC} \end{pmatrix}, \quad S = \begin{pmatrix} S_{AA} & S_{AB} & S_{AC} \\ S_{BA} & S_{BB} & S_{BC} \\ S_{CA} & S_{CB} & S_{CC} \end{pmatrix}. \quad (2.11)$$

To determine the explicit expressions of these matrix elements, we first consider the contribution arising from the A and B sites. In this case, the corresponding transfer integral (hopping) matrix element is given by

$$H_{AB} = \frac{1}{N} \sum_{\mathbf{R}'_i, \mathbf{R}_i} e^{i\mathbf{k} \cdot (\mathbf{R}'_i - \mathbf{R}_i)} t_{\mathbf{R}'_i, \mathbf{R}_i}^{AB}, \quad (2.12)$$

where only first-nearest-neighbor contributions are retained. Denoting $t \equiv t_{\mathbf{R}'_i, \mathbf{R}_i}^{AB}$ and noting that each A site is coupled to three B sites, one obtains

$$H_{AB} = \frac{1}{N} \left(Nt \sum_{n=1}^3 e^{i\mathbf{k} \cdot \mathbf{d}_n} \right), \quad (2.13)$$

where $\mathbf{d}_1 = (a, 0)$, $\mathbf{d}_2 = (-a/2, a\sqrt{3}/2)$, and $\mathbf{d}_3 = (-a/2, -a\sqrt{3}/2)$, as illustrated in Fig. 16. This leads to

$$H_{AB} = t \left[e^{ik_x a} + 2e^{\frac{-ik_x a}{2}} \cos \left(\frac{k_y \sqrt{3}a}{2} \right) \right] = H_{BA}^*. \quad (2.14)$$

For the overlap between sites A and B , the corresponding matrix element is

$$S_{AB} = \frac{1}{N} \sum_{\mathbf{R}'_i, \mathbf{R}_i} e^{i\mathbf{k} \cdot (\mathbf{R}'_i - \mathbf{R}_i)} s_{\mathbf{R}'_i, \mathbf{R}_i}^{AB}, \quad (2.15)$$

and, proceeding analogously to the previous derivation and again restricting to first-nearest neighbors, we obtain

$$S_{AB} = \frac{1}{N} \left(N_s \sum_{n=1}^3 e^{i\mathbf{k} \cdot \mathbf{d}_n} \right) = s \left[e^{ik_x a} + 2e^{\frac{-ik_x a}{2}} \cos \left(\frac{k_y \sqrt{3}a}{2} \right) \right] = S_{BA}^*. \quad (2.16)$$

From Fig. 16, the transfer integrals satisfy the relations $H_{AB}/t = H_{CA}/\alpha t_A = H_{BC}/\alpha t_B$, and for the overlap elements one has $S_{BC} = S_{CA} = S_{AB}$ and $S_{AC} = S_{CB} = S_{AB}^*$. For the onsite terms of the transfer integral (onsite energies), we define $H_{jj} = \epsilon_j$, and for the overlap matrix we set $S_{jj} = 1$ ($j = \{A, B, C\}$). Consequently, the matrices in Eq. (2.11) take the form

$$H = \begin{pmatrix} \epsilon_A & tf(\mathbf{k}) & \alpha t_A f^*(\mathbf{k}) \\ tf^*(\mathbf{k}) & \epsilon_B & \alpha t_B f(\mathbf{k}) \\ \alpha t_A f(\mathbf{k}) & \alpha t_B f^*(\mathbf{k}) & \epsilon_C \end{pmatrix} \quad S = \begin{pmatrix} 1 & sf(\mathbf{k}) & s_A f^*(\mathbf{k}) \\ sf^*(\mathbf{k}) & 1 & s_B f(\mathbf{k}) \\ s_A f(\mathbf{k}) & s_B f^*(\mathbf{k}) & 1 \end{pmatrix}, \quad (2.17)$$

where the lattice structure factor is defined as

$$f(\mathbf{k}) = \left[e^{ik_x a} + 2e^{\frac{-ik_x a}{2}} \cos \left(\frac{k_y \sqrt{3}a}{2} \right) \right]. \quad (2.18)$$

To determine the energy bands of the lattice, we introduce the parametrization $\alpha = \tan \theta$ and rescale the hopping sector of the Hamiltonian as follows:

$$H = \begin{pmatrix} \epsilon_A & tf(\mathbf{k}) & \alpha t_A f^*(\mathbf{k}) \\ tf^*(\mathbf{k}) & \epsilon_B & \alpha t_B f(\mathbf{k}) \\ \alpha t_A f(\mathbf{k}) & \alpha t_B f^*(\mathbf{k}) & \epsilon_C \end{pmatrix} = \underbrace{\begin{pmatrix} \epsilon_A & 0 & 0 \\ 0 & \epsilon_B & 0 \\ 0 & 0 & \epsilon_C \end{pmatrix}}_{H_0} + \underbrace{\begin{pmatrix} 0 & tf(\mathbf{k}) & \alpha t_A f^*(\mathbf{k}) \\ tf^*(\mathbf{k}) & 0 & \alpha t_B f(\mathbf{k}) \\ \alpha t_A f(\mathbf{k}) & \alpha t_B f^*(\mathbf{k}) & 0 \end{pmatrix}}_{H_h}. \quad (2.19)$$

The rescaled Hamiltonian is then defined by $H_\theta = H_0 + \cos \theta H_h$ ², so that the energy spectrum is obtained from the generalized eigenvalue problem

$$\det[H_\theta - ES] = 0, \quad (2.20)$$

² H_0 (onsite contribution), H_h (hopping contribution).

where

$$H_\theta = \begin{pmatrix} \epsilon_A & \cos \theta t f(\mathbf{k}) & \sin \theta t_A f^*(\mathbf{k}) \\ \cos \theta t f^*(\mathbf{k}) & \epsilon_B & \sin \theta t_B f(\mathbf{k}) \\ \sin \theta t_A f(\mathbf{k}) & \sin \theta t_B f^*(\mathbf{k}) & \epsilon_C \end{pmatrix}. \quad (2.21)$$

For an orthogonal TB basis, the overlap matrix S is the identity. We now evaluate the band structure for the parameter choice $\epsilon_A = \epsilon_B = \epsilon_C = \epsilon$, $t_A = 0$, $t_B = t$, which yields

$$\det[H_\theta - EI] = \begin{vmatrix} \epsilon - E & \cos \theta t f(\mathbf{k}) & 0 \\ \cos \theta t f^*(\mathbf{k}) & \epsilon - E & \sin \theta t f(\mathbf{k}) \\ 0 & \sin \theta t f^*(\mathbf{k}) & \epsilon - E \end{vmatrix} = 0. \quad (2.22)$$

Solving this equation leads to the eigenvalues

$$E(\mathbf{k}) = \epsilon, \quad E_\pm(\mathbf{k}) = \epsilon \mp t|f(\mathbf{k})|. \quad (2.23)$$

The resulting dispersion relation thus consists of three bands, each accounting for one-third of the total states: one nondispersive (flat) band at $E = \epsilon$, and two dispersive bands that correspond to the conduction and valence bands of graphene-like character, exhibiting electron-hole symmetry. Within this rescaled model and for an orthogonal TB description (*i.e.*, neglecting orbital overlap³), the spectrum is independent of the choice of the morphological angle θ .

2.3 The Tight-Binding Model for $\alpha - T_3$ Lattice in the Second Quantization

In order to transition from the first-quantized to the second-quantized formalism, one typically begins with a generic additive one-body operator,

$$J = \sum_i J(x_i), \quad (2.24)$$

where the sum runs over all particles (LIMA *et al.*, 2022). This is precisely the situation encountered in the first-quantization framework when we assume that the eigenvalues and eigenfunctions of the Schrödinger equation for an isolated atom define a set of atomic orbitals that can be used as an approximate basis for the electronic states in a crystalline solid. Under this assumption, Bloch functions are constructed from these localized atomic orbitals as appropriate linear combinations.

³ Tight-binding model without orbital-overlap matrix elements.

The representation of J in Eq. (2.24) is referred to as first quantization (COTTAM; HAGHSHENASFARD, 2020). In second quantization, the same operator is expressed as

$$J = \sum_{ij} \langle i | J | j \rangle \hat{a}_i^\dagger \hat{a}_j, \quad (2.25)$$

where $\hat{a}_i^\dagger$ and $\hat{a}_j$ are the fermionic (or bosonic, as appropriate) creation and annihilation operators associated with the single-particle states $|i\rangle$ and $|j\rangle$ (SAKURAI; NAPOLITANO, 2020), respectively.

Neglecting electron–electron interactions, a general single-particle Hamiltonian in second quantization can be written by identifying $J = H$:

$$\hat{H} = \sum_{ij} \langle i | H | j \rangle \hat{a}_i^\dagger \hat{a}_j. \quad (2.26)$$

Here, i and j label generic single-particle states. For $i = j$, we define the on-site energy

$$E_i = \langle i | H | i \rangle,$$

whereas for $i \neq j$ we define the hopping (transfer) amplitude

$$t_{ij} = \langle i | H | j \rangle.$$

Equation (2.26) is fully analogous to Eq. (2.8). Consequently, the TB description in the second-quantized formalism embodies the same physical content and assumptions as the corresponding first-quantized model. The crucial difference is that, instead of being expressed in terms of Bloch functions, the theory is formulated in terms of creation and annihilation operators acting on Fock space (LIMA, 2020; COTTAM; HAGHSHENASFARD, 2020).

The TB Hamiltonian—cleanly splitting the local on-site energy terms, which capture the unique electronic environment at each atomic site, from the hopping terms, which describe electron transfer between neighboring sites—takes the form

$$\hat{H} = \sum_i \epsilon_i \hat{n}_i + \sum_{i \neq j} t_{ij} \hat{g}_i^\dagger \hat{g}_j + h.c. \quad (2.27)$$

where $h.c.$ denotes the Hermitian conjugate, and the remaining quantities are defined as follows:

- ϵ_i is the on-site energy at the i th atomic site;

- $\hat{n}_i = \hat{g}_i^\dagger \hat{g}_i$ is the number operator, which counts the electrons at the i th atomic site;
- t_{ij} is the hopping amplitude (transfer integral) between atomic sites i and j ;
- $\hat{g}_i^\dagger$ ($\hat{g}_i$) is the creation (annihilation) operator for an electron or a hole at the i th atomic site.

Focusing on the first term in Eq. (2.27), the crystalline lattice is assumed to decompose into three inequivalent sublattices. Consequently, one can rewrite

$$\sum_i \epsilon_i \hat{n}_i = \sum_i \epsilon_A \hat{a}_i^\dagger \hat{a}_i + \sum_i \epsilon_B \hat{b}_i^\dagger \hat{b}_i + \sum_i \epsilon_C \hat{c}_i^\dagger \hat{c}_i, \quad (2.28)$$

where ϵ_m denotes the on-site energy associated with sublattice $m = \{A, B, C\}$, and $\hat{a}_i^\dagger, \hat{b}_i^\dagger, \hat{c}_i^\dagger$ ($\hat{a}_i, \hat{b}_i, \hat{c}_i$) are the corresponding electron creation (annihilation) operators at the i th atomic site of sublattices A, B , and C , respectively. In Eq. (2.28), each summation is restricted to the set of atomic sites i belonging to the corresponding sublattice.

Since the crystalline lattice is periodic and infinite, it is convenient to perform a Fourier transformation of the creation and annihilation operators:

$$\hat{g}_i^\dagger = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\mathbf{k} \cdot \mathbf{r}_i} \hat{g}_{\mathbf{k}}^\dagger, \quad (2.29)$$

$$\hat{g}_i = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{r}_i} \hat{g}_{\mathbf{k}}, \quad (2.30)$$

where $g = \{a, b, c\}$, N denotes the total number of unit cells in the crystalline lattice, $\hat{g}_{\mathbf{k}}^\dagger$ ($\hat{g}_{\mathbf{k}}$) creates (annihilates) an electron with wave vector $\mathbf{k}$ in reciprocal space, and $\mathbf{r}_i$ is the position of the i -th atomic site of the corresponding sublattice. For instance, if $g = a$, then $\mathbf{r}_i$ refers to the position of the i -th atomic site belonging to sublattice A .

To diagonalize the TB Hamiltonian, we substitute Eqs. (2.29) and (2.30) into Eq. (2.28), obtaining

$$\begin{aligned} \hat{H}_\epsilon = & \epsilon_A \sum_i \frac{1}{N} \sum_{\mathbf{k}, \mathbf{k}'} e^{-i(\mathbf{k}' - \mathbf{k}) \cdot \mathbf{r}_i} \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}'} + \epsilon_B \sum_i \frac{1}{N} \sum_{\mathbf{k}, \mathbf{k}'} e^{-i(\mathbf{k}' - \mathbf{k}) \cdot \mathbf{r}_i} \hat{b}_{\mathbf{k}}^\dagger \hat{b}_{\mathbf{k}'} \\ & + \epsilon_C \sum_i \frac{1}{N} \sum_{\mathbf{k}, \mathbf{k}'} e^{-i(\mathbf{k}' - \mathbf{k}) \cdot \mathbf{r}_i} \hat{c}_{\mathbf{k}}^\dagger \hat{c}_{\mathbf{k}'}, \end{aligned} \quad (2.31)$$

which, after permuting the order of summation, can be written as

$$\begin{aligned} \hat{H}_\epsilon = & \epsilon_A \sum_{\mathbf{k}, \mathbf{k}'} \sum_i \frac{1}{N} e^{-i(\mathbf{k}' - \mathbf{k}) \cdot \mathbf{r}_i} \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}'} + \epsilon_B \sum_{\mathbf{k}, \mathbf{k}'} \sum_i \frac{1}{N} e^{-i(\mathbf{k}' - \mathbf{k}) \cdot \mathbf{r}_i} \hat{b}_{\mathbf{k}}^\dagger \hat{b}_{\mathbf{k}'} \\ & + \epsilon_C \sum_{\mathbf{k}, \mathbf{k}'} \sum_i \frac{1}{N} e^{-i(\mathbf{k}' - \mathbf{k}) \cdot \mathbf{r}_i} \hat{c}_{\mathbf{k}}^\dagger \hat{c}_{\mathbf{k}'}. \end{aligned} \quad (2.32)$$

Exploiting the orthogonality relation in reciprocal space, we have

$$\sum_i \frac{1}{N} e^{-i(\mathbf{k}' - \mathbf{k}) \cdot \mathbf{r}_i} = \delta_{\mathbf{k}, \mathbf{k}'}, \quad (2.33)$$

so that Eq. (2.32) reduces to

$$\hat{H}_\epsilon = \sum_{\mathbf{k}} \epsilon_A \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} + \sum_{\mathbf{k}} \epsilon_B \hat{b}_{\mathbf{k}}^\dagger \hat{b}_{\mathbf{k}} + \sum_{\mathbf{k}} \epsilon_C \hat{c}_{\mathbf{k}}^\dagger \hat{c}_{\mathbf{k}}. \quad (2.34)$$

In matrix form, this on-site contribution to the Hamiltonian can be expressed as

$$\hat{H}_\epsilon = \sum_{\mathbf{k}} \begin{pmatrix} \hat{a}_{\mathbf{k}}^\dagger & \hat{b}_{\mathbf{k}}^\dagger & \hat{c}_{\mathbf{k}}^\dagger \end{pmatrix} \begin{pmatrix} \epsilon_A & 0 & 0 \\ 0 & \epsilon_B & 0 \\ 0 & 0 & \epsilon_C \end{pmatrix} \begin{pmatrix} \hat{a}_{\mathbf{k}} \\ \hat{b}_{\mathbf{k}} \\ \hat{c}_{\mathbf{k}} \end{pmatrix}. \quad (2.35)$$

We now focus on the second term of Eq. (2.27), which in our case reads

$$\sum_{i \neq j} t_{ij} g_i^\dagger g_j + \text{h.c.} = \sum_{i,j} t (\hat{a}_i^\dagger \hat{b}_j + \hat{b}_j^\dagger \hat{a}_i) + \sum_{j,l} \alpha t_A (\hat{a}_j^\dagger \hat{c}_l + \hat{c}_l^\dagger \hat{a}_j) + \sum_{l,m} \alpha t_B (\hat{b}_l^\dagger \hat{c}_m + \hat{c}_m^\dagger \hat{b}_l). \quad (2.36)$$

According to Eqs. (2.29) and (2.30), for the hopping process $A \rightarrow B$ (creation on site A and annihilation on site B), we obtain

$$\sum_{i,j} t (\hat{a}_i^\dagger \hat{b}_j) = t \sum_{i,j} \left(\frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\mathbf{k} \cdot \mathbf{r}_i} \hat{a}_{\mathbf{k}}^\dagger \right) \left(\frac{1}{\sqrt{N}} \sum_{\mathbf{k}'} e^{i\mathbf{k}' \cdot \mathbf{r}_j} \hat{b}_{\mathbf{k}'} \right), \quad (2.37)$$

which, upon permutation of the summation indices, can be recast as

$$\sum_{i,j} t (\hat{a}_i^\dagger \hat{b}_j) = \sum_{\mathbf{k}, \mathbf{k}'} \frac{t}{N} \sum_{i,j} (e^{-i\mathbf{k} \cdot \mathbf{r}_i} e^{i\mathbf{k}' \cdot \mathbf{r}_j}) (e^{-i\mathbf{k}' \cdot \mathbf{r}_i} e^{i\mathbf{k} \cdot \mathbf{r}_j}) \hat{a}_{\mathbf{k}}^\dagger \hat{b}_{\mathbf{k}'}, \quad (2.38)$$

which in turn can be rewritten in the more compact form

$$\sum_{i,j} t (\hat{a}_i^\dagger \hat{b}_j) = t \sum_{\mathbf{k}, \mathbf{k}'} \frac{1}{N} \sum_{i,j} e^{i(\mathbf{k}' - \mathbf{k}) \cdot \mathbf{r}_i} e^{-i\mathbf{k}' \cdot \mathbf{d}_{ij}} \hat{a}_{\mathbf{k}}^\dagger \hat{b}_{\mathbf{k}'}, \quad (2.39)$$

where $\mathbf{d}_{ij} = \mathbf{r}_i - \mathbf{r}_j$ denotes the position of the sublattice A with respect to sublattice B .

We now keep the index i fixed and perform the summation over the index j , yielding

$$\sum_{i,j} t (\hat{a}_i^\dagger \hat{b}_j) = t \sum_{\mathbf{k}, \mathbf{k}'} \underbrace{\sum_i \frac{1}{N} e^{i(\mathbf{k}' - \mathbf{k}) \cdot \mathbf{r}_i}}_{=\delta_{\mathbf{k}, \mathbf{k}'}} \sum_{n=1}^3 e^{i\mathbf{k}' \cdot \mathbf{d}_n} \hat{a}_{\mathbf{k}}^\dagger \hat{b}_{\mathbf{k}'} = t \sum_{\mathbf{k}} f(\mathbf{k}) \hat{a}_{\mathbf{k}}^\dagger \hat{b}_{\mathbf{k}}, \quad (2.40)$$

that is,

$$\sum_{i,j} t(\hat{a}_i^\dagger \hat{b}_j) = t \sum_{\mathbf{k}} f(\mathbf{k}) \hat{a}_{\mathbf{k}}^\dagger \hat{b}_{\mathbf{k}}, \quad (2.41)$$

with $f(\mathbf{k}) = \sum_{n=1}^3 e^{i\mathbf{k} \cdot \mathbf{d}_n}$. From Fig. 16 we have $\mathbf{d}_1 = (a, 0)$, $\mathbf{d}_2 = (-a/2, a\sqrt{3}/2)$ and $\mathbf{d}_3 = (-a/2, -a\sqrt{3}/2)$, which leads to

$$f(\mathbf{k}) = \left[e^{ik_x a} + 2e^{-ik_x a/2} \cos\left(\frac{k_y \sqrt{3}a}{2}\right) \right]. \quad (2.42)$$

For the reverse hopping $B \rightarrow A$, we obtain in an analogous manner

$$\sum_{i,j} t(\hat{b}_j^\dagger \hat{a}_i) = t \sum_{\mathbf{k}} f^*(\mathbf{k}) \hat{b}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}}, \quad (2.43)$$

while the processes $B \rightarrow C$ ($C \rightarrow A$) are equivalent to the case $A \rightarrow B$, up to the multiplicative constants t_A (t_B), respectively. By the same reasoning applied to $C \rightarrow B$ ($A \rightarrow C$) and $B \rightarrow A$, we obtain

$$\begin{aligned} \sum_{i \neq j} t_{ij} g_i^\dagger g_j &= \sum_{\mathbf{k}} t [f(\mathbf{k}) \hat{a}_{\mathbf{k}}^\dagger \hat{b}_{\mathbf{k}} + f^*(\mathbf{k}) \hat{b}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}}] + \sum_{\mathbf{k}} \alpha t_B [f(\mathbf{k}) \hat{b}_{\mathbf{k}}^\dagger \hat{c}_{\mathbf{k}} + f^*(\mathbf{k}) \hat{c}_{\mathbf{k}}^\dagger \hat{b}_{\mathbf{k}}] + \\ &+ \sum_{\mathbf{k}} \alpha t_A [f(\mathbf{k}) \hat{b}_{\mathbf{k}}^\dagger \hat{c}_{\mathbf{k}} + f^*(\mathbf{k}) \hat{c}_{\mathbf{k}}^\dagger \hat{b}_{\mathbf{k}}], \end{aligned} \quad (2.44)$$

which can be expressed in matrix form as

$$\sum_{i \neq j} t_{ij} g_i^\dagger g_j = \sum_{\mathbf{k}} \begin{pmatrix} \hat{a}_{\mathbf{k}}^\dagger & \hat{b}_{\mathbf{k}}^\dagger & \hat{c}_{\mathbf{k}}^\dagger \end{pmatrix} \begin{pmatrix} 0 & tf(\mathbf{k}) & \alpha t_A f^*(\mathbf{k}) \\ tf^*(\mathbf{k}) & 0 & \alpha t_B f(\mathbf{k}) \\ \alpha t_A f(\mathbf{k}) & \alpha t_B f^*(\mathbf{k}) & 0 \end{pmatrix} \begin{pmatrix} \hat{a}_{\mathbf{k}} \\ \hat{b}_{\mathbf{k}} \\ \hat{c}_{\mathbf{k}} \end{pmatrix}. \quad (2.45)$$

Combining Eqs. (2.35) and (2.45), the Hamiltonian operator in momentum space is given by

$$H = \begin{pmatrix} \epsilon_A & tf(\mathbf{k}) & \alpha t_A f^*(\mathbf{k}) \\ tf^*(\mathbf{k}) & \epsilon_B & \alpha t_B f(\mathbf{k}) \\ \alpha t_A f(\mathbf{k}) & \alpha t_B f^*(\mathbf{k}) & \epsilon_C \end{pmatrix}. \quad (2.46)$$

Analogously to the first-quantization treatment, we diagonalize the rescaled Hamiltonian in order to determine the energy bands of the lattice. Here, however, we consider the specific situation in which there is a bond between sites A and C ($t_A = t$ and $t_B = 0$), so that

$$\det[H_\theta - EI] = \begin{vmatrix} \epsilon - E & \cos \theta tf(\mathbf{k}) & \sin \theta tf^*(\mathbf{k}) \\ \cos \theta tf^*(\mathbf{k}) & \epsilon - E & 0 \\ \sin \theta tf(\mathbf{k}) & 0 & \epsilon - E \end{vmatrix}, \quad (2.47)$$

which yields the eigenvalues

$$E(\mathbf{k}) = \epsilon \quad \text{and} \quad E_{\pm}(\mathbf{k}) = \epsilon \mp t|f(\mathbf{k})|. \quad (2.48)$$

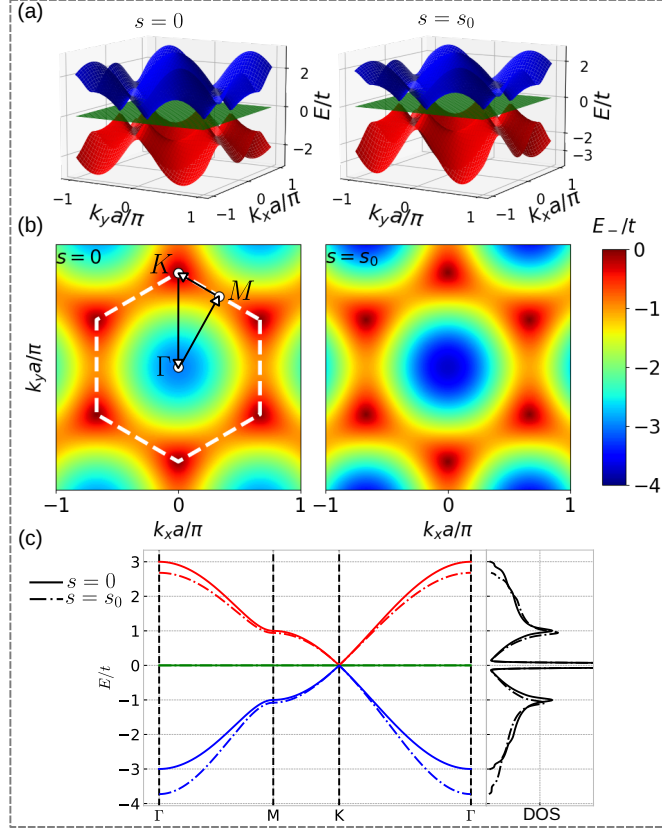
Therefore, the TB description in second quantization is equivalent to the orthogonal TB formulation in first quantization. Moreover, the energy dispersion is identical for the two limiting cases $t_A = 0$, $t_B = t$ and $t_A = t$, $t_B = 0$. In the next section, we will present the numerical results for the energy bands and the density of states (DOS).⁴

2.4 Energy Dispersion of the $\alpha - T_3$ Model

The energy dispersion relations and the corresponding Density of states (DOS) of the $\alpha - T_3$ lattice, computed within the framework of the TB model using both first- and second-quantization formalisms, are presented in Fig. 18.

⁴ The DOS is evaluated by superposing the individual energy levels, broadened by a Gaussian function $f(E) = e^{-(E-E_0)/\gamma^2}$ with a broadening parameter $\gamma = 0.05$ eV, chosen smaller than the typical level spacing; see Ref. (LIMA *et al.*, 2022).

Figure 18 – Band structure of the lattice $\alpha - T_3$. In (a) there is the complete band structure, in (b) the contour of the valence band, and in (c) is the band structure at points of high symmetry and its respective density of states (DOS), with continuous lines corresponding to the overlap value $s = 0$ and dotted lines corresponding to the overlap value $s_0 = 0.065$.



Source: The author.

The dispersion relation of $\alpha - T_3$ within an orthogonal TB framework is identical to the conduction and valence band structure of graphene. However, in addition to these dispersive bands, the spectrum contains a flat, nondispersive band that intersects the Dirac points, i.e., the points at which the conduction and valence bands meet. Moreover, the presence of this nondispersive band at $E = 0$ gives rise to an enhanced DOS in the vicinity of this energy. In contrast, the nonorthogonal TB model explicitly incorporates orbital overlap, thereby breaking electron-hole symmetry and introducing a dependence of the band structure on the morphological angle θ .

2.5 Continuum Model for $\alpha - T_3$ Lattice

For a continuum description, we expand the lattice structure factor $f(\mathbf{k})$ in a Taylor series around the inequivalent Dirac points K and K' , as is standard in the

treatment of graphene. From the literature, it is well established that the low-energy TB Hamiltonian of graphene can be expressed in terms of Pauli matrices as

$$H_{\text{graphene}} = v_f \boldsymbol{\sigma} \cdot \mathbf{p}, \quad (2.49)$$

where $\boldsymbol{\sigma}$ denotes the usual vector of Pauli spin matrices,

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (2.50)$$

Thus, the effective Hamiltonian for graphene corresponds to a pseudospin- $S = 1/2$ system. Moreover, the Pauli matrices satisfy the usual angular momentum commutation relations

$$[\sigma_i, \sigma_j] = i\epsilon_{ijk}\sigma_k, \quad (2.51)$$

as well as the Clifford algebra

$$\{\sigma_i, \sigma_j\} = 2\delta_{ij}I, \quad (2.52)$$

where I is the 2×2 identity matrix (URBAN *et al.*, 2011). The corresponding energy dispersion relation is

$$E = \pm v_f p, \quad (2.53)$$

which is linear in the momentum magnitude $p = |\mathbf{p}|$.

This linear dispersion implies that low-energy charge carriers in graphene propagate with a constant group velocity v_f , analogous to massless relativistic particles, for which v_f plays the role of an effective speed of light. In so-called Dirac materials, these low-energy fermionic excitations (quasiparticles) are therefore not governed by the conventional Schrödinger Hamiltonian, $H = \mathbf{p}^2/2m^*$, but instead by a Dirac-type Hamiltonian (WAKABAYASHI *et al.*, 2010) of the form

$$H = c \boldsymbol{\sigma} \cdot \mathbf{p} + mc^2 \sigma_z. \quad (2.54)$$

In the limit of vanishing Dirac mass, $m \rightarrow 0$, this Hamiltonian reduces to the effective low-energy TB Hamiltonian of graphene, with the effective “speed of light” c identified with the Fermi velocity v_f . In graphene, this Fermi velocity is approximately $v_f \approx 3 \times 10^6$ m/s (HWANG *et al.*, 2012).

To obtain the low-energy $\alpha - T_3$ Hamiltonian, we expand the lattice structure factor $f(\mathbf{k})$ in a Taylor series around the inequivalent Dirac points K and K' as

$$f(\mathbf{k}) = f(0, K) + k_x \left. \frac{\partial f}{\partial k_x} \right|_{k_x=0} + (k_y - K) \left. \frac{\partial f}{\partial k_y} \right|_{k_y=K} + \dots, \quad (2.55)$$

where

$$f(\mathbf{k}) = e^{ik_x a} + 2e^{-ik_x a/2} \cos\left(\frac{k_y \sqrt{3}a}{2}\right). \quad (2.56)$$

In the low-energy regime, the expansion can be written more compactly as

$$f(\mathbf{k}) \approx f(\mathbf{k})|_{\mathbf{k}=\xi K} + k_x \left. \frac{\partial f}{\partial k_x} \right|_{\mathbf{k}=\xi K} + (k_y - K) \left. \frac{\partial f}{\partial k_y} \right|_{\mathbf{k}=\xi K}, \quad (2.57)$$

which yields

$$f(\mathbf{k} + \xi K) = i \frac{3a}{2} (k_x + \xi i k_y) = e^{i\pi/2} \frac{3a}{2} (k_x + \xi i k_y). \quad (2.58)$$

Since the global phase factor does not have physical consequences, we may redefine

$$f(\mathbf{k} + \xi K) = \frac{3a}{2} (k_x + \xi i k_y), \quad (2.59)$$

where $\xi = 1 (-1)$ labels the $K (K')$ valley, respectively. Substituting this into the TB Hamiltonian (2.46) and retaining only the low-energy contributions, we obtain

$$H_\theta = \begin{pmatrix} \epsilon_A & \cos \theta \frac{3at}{2} (k_x + \xi i k_y) & \sin \theta \frac{3at_A}{2} (k_x - \xi i k_y) \\ \cos \theta \frac{3at}{2} (k_x - \xi i k_y) & \epsilon_B & \sin \theta \frac{3at_B}{2} (k_x + \xi i k_y) \\ \sin \theta \frac{3at_A}{2} (k_x + \xi i k_y) & \sin \theta \frac{3at_B}{2} (k_x - \xi i k_y) & \epsilon_C \end{pmatrix}. \quad (2.60)$$

We now focus on the special cases $t_B = t$, $t_A = 0$ and $t_B = 0$, $t_A = t$, setting $\epsilon_j = 0$ for $j = \{A, B, C\}$ in both situations. First, we note that the prefactor $3at/2$ has the dimension of $\hbar v_f$, where v_f denotes the Fermi velocity (ILLES, 2017). Accordingly, the Hamiltonian for the case $t_B = t$, $t_A = 0$ can be written as

$$H_\theta|_{t_B=t, t_A=0} = \hbar v_f \begin{pmatrix} 0 & \cos \theta (k_x + \xi i k_y) & 0 \\ \cos \theta (k_x - \xi i k_y) & 0 & \sin \theta (k_x + \xi i k_y) \\ 0 & \sin \theta (k_x - \xi i k_y) & 0 \end{pmatrix}. \quad (2.61)$$

This Hamiltonian can be decomposed into a linear combination of basis matrices as

$$H_\theta = \hbar v_f k_x \begin{pmatrix} 0 & \cos \theta & 0 \\ \cos \theta & 0 & \sin \theta \\ 0 & \sin \theta & 0 \end{pmatrix} + \xi i \hbar v_f k_y \begin{pmatrix} 0 & \cos \theta & 0 \\ -\cos \theta & 0 & \sin \theta \\ 0 & -\sin \theta & 0 \end{pmatrix}, \quad (2.62)$$

which can be written in the compact form

$$H_\theta = \hbar v_f \mathbf{S} \cdot \mathbf{k}, \quad (2.63)$$

where the pseudospin-1 matrices are given by

$$S_x = \begin{pmatrix} 0 & \cos \theta & 0 \\ \cos \theta & 0 & \sin \theta \\ 0 & \sin \theta & 0 \end{pmatrix}, \quad S_y = \xi \begin{pmatrix} 0 & i \cos \theta & 0 \\ -i \cos \theta & 0 & i \sin \theta \\ 0 & -i \sin \theta & 0 \end{pmatrix}. \quad (2.64)$$

For the complementary case $t_B = 0$, $t_A = t$, and under the same low-energy and on-site energy assumptions, the effective Hamiltonian can similarly be expressed as

$$H_\theta = \hbar v_f \mathbf{S}' \cdot \mathbf{k}, \quad (2.65)$$

with the corresponding pseudospin matrices

$$S'_x = \begin{pmatrix} 0 & \cos \theta & \sin \theta \\ \cos \theta & 0 & 0 \\ \sin \theta & 0 & 0 \end{pmatrix}, \quad S'_y = \xi \begin{pmatrix} 0 & i \cos \theta & -i \sin \theta \\ -i \cos \theta & 0 & 0 \\ i \sin \theta & 0 & 0 \end{pmatrix}. \quad (2.66)$$

We now analyze the limiting values of the morphological angle θ . For $\theta = 0$, the model reduces to a graphene-like system, up to the presence of an additional zero-energy flat band arising from the decoupled C sites. In this limit, the pseudospin matrices in Eqs. (2.64) and (2.66) become essentially equivalent and can be cast into the Dirac–Weyl form (RAOUX *et al.*, 2014), yielding

$$H_0 = \hbar v_f \boldsymbol{\sigma} \cdot \mathbf{k} \oplus 0. \quad (2.67)$$

Thus, the $\alpha - T_3$ model reproduces the graphene Dirac Hamiltonian, despite the enlarged unit cell with three inequivalent sites.

In the opposite limit, $\theta = \pi/4$, the pseudospin matrices (2.64) and (2.66) no longer coincide and must be treated separately. The matrices (2.64) at $\theta = \pi/4$ realize a pseudospin-1 representation, i.e., they furnish a three-dimensional irreducible representation of $SU(2)$ and satisfy the standard angular-momentum commutation relations

$$[S_m, S_n] = i\epsilon_{mnl} S_l. \quad (2.68)$$

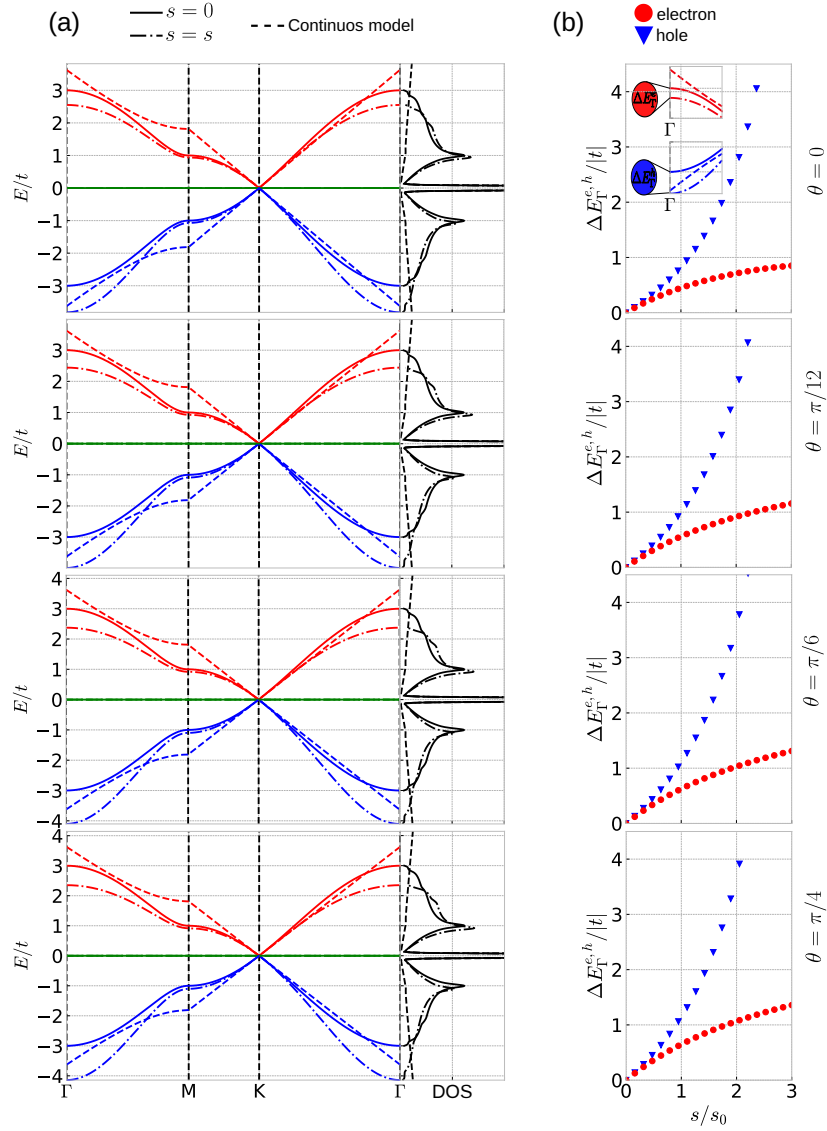
However, unlike the Pauli matrices, these spin-1 operators do not generate a Clifford algebra; specifically,

$$\{S_n, S_m\} \neq 2\delta_{n,m} I_3 \quad (2.69)$$

(URBAN *et al.*, 2011). In contrast, the matrices (2.66) evaluated at $\theta = \pi/4$ fail to satisfy both the angular-momentum commutation relations and the Clifford algebra.

In summary, the rescaled $\alpha - T_3$ model with hopping amplitudes $t_A = 0$ and $t_B = t$ (see Fig. 16) implements a continuous interpolation between massless Dirac quasiparticles with pseudospin $S = 1/2$ at $\theta = 0$ and massless fermions with pseudospin $S = 1$ at $\theta = \pi/4$ (BETANCUR-OCAMPO *et al.*, 2017). Figure 19 compares the TB band structure with the corresponding low-energy continuum description at the high-symmetry points of the Brillouin zone.

Figure 19 – Band structures at high-symmetry points for different values of the morphological angle $\theta = \tan^{-1} \alpha$ are shown for $\theta = 0$, $\theta = \pi/12$, $\theta = \pi/6$, and $\theta = \pi/4$, together with the corresponding densities of states (DOS). In panel (a), solid curves represent the case without orbital overlap ($s = 0$), dashed curves correspond to the continuum model, and dash-dotted curves represent the band structure including a finite overlap $s_0 = 0.065$. Panel (b) displays, for each value of the morphological angle θ , the absolute difference between the valence (hole) and conduction (electron) energy bands obtained with ($s = s_0$) and without ($s = 0$) orbital overlap as a function of the overlap parameter s at the Γ point.



Source: The author.

In the vicinity of the K valley in Figs. 19(a), the continuum model provides an accurate approximation. This framework enables the analysis of low-energy excitations by employing the relativistic high-energy formalism encoded in the Dirac equation (WEHLING *et al.*, 2014).

As previously demonstrated (see Fig. 18), the inclusion of orbital overlap breaks electron–hole symmetry. However, the nature and magnitude of this symmetry breaking differ between transition lattices and among the high-symmetry points Γ , M , and K . In Fig. 19(b), which displays the difference between overlapping and orthogonal orbitals for the electron and hole states at the high-symmetry point Γ , one observes that the hole state (valence band) is more strongly affected than the electron state (conduction band) as the orbital overlap increases.

It is important to emphasize that, to the best of our knowledge, a systematic treatment of non-orthogonal orbitals in the $\alpha - T_3$ lattice, particularly for transition cases, is absent from the existing literature.

2.6 Wavefunctions of the $\alpha - T_3$ Lattice

In the previous section, we determined the energy eigenvalues associated with the lattice $\alpha - T_3$ Hamiltonian in Eq. (2.46). We now proceed to obtain the corresponding eigenvectors by solving the time-independent Schrödinger equation

$$H(\mathbf{k})|\psi\rangle = E_{\mathbf{k}}|\psi\rangle. \quad (2.70)$$

We first consider the dispersive bands, for which $E_{\mathbf{k}} = \pm t |f(\mathbf{k})|$. In the sublattice basis, the state $|\psi\rangle$ can be represented as

$$|\psi\rangle \doteq \begin{pmatrix} a \\ b \\ c \end{pmatrix}, \quad (2.71)$$

so that Eq. (2.70) acquires the matrix form

$$\begin{pmatrix} 0 & \cos \theta f(\mathbf{k}) & 0 \\ \cos \theta f^*(\mathbf{k}) & 0 & \sin \theta f(\mathbf{k}) \\ 0 & \sin \theta f^*(\mathbf{k}) & 0 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = E_k \begin{pmatrix} a \\ b \\ c \end{pmatrix}. \quad (2.72)$$

This leads to the coupled equations

$$b f(\mathbf{k}) \cos \theta = a E_k, \quad (2.73)$$

$$a f^*(\mathbf{k}) \cos \theta + c f(\mathbf{k}) \sin \theta = b E_k, \quad (2.74)$$

$$b f^*(\mathbf{k}) \sin \theta = c E_k. \quad (2.75)$$

Multiplying Eqs. (2.73), (2.74), and (2.75) by a^* , b^* , and c^* , respectively, we obtain

$$a^* b f(\mathbf{k}) \cos \theta = |a|^2 E_k, \quad (2.76)$$

$$b^* a f^*(\mathbf{k}) \cos \theta + b^* c f(\mathbf{k}) \sin \theta = |b|^2 E_k, \quad (2.77)$$

$$c^* b f^*(\mathbf{k}) \sin \theta = |c|^2 E_k. \quad (2.78)$$

Since the right-hand sides of Eqs. (2.76)–(2.78) are real, we may combine them by substituting Eqs. (2.76) and (2.78) into Eq. (2.77), which yields the relation

$$|a|^2 + |c|^2 = |b|^2. \quad (2.79)$$

Imposing the normalization condition on $|\psi\rangle$, namely $\langle\psi|\psi\rangle = 1$, we obtain an additional constraint,

$$|a|^2 + |b|^2 + |c|^2 = 1. \quad (2.80)$$

Solving Eqs. (2.79) and (2.80) simultaneously, we find

$$|b| = \frac{1}{\sqrt{2}}, \quad (2.81)$$

so that $b = \pm 1/\sqrt{2}$ up to an overall phase. Substituting this result into Eqs. (2.73) and (2.75), we obtain

$$a = \pm \frac{f(\mathbf{k})}{E_k \sqrt{2}} \cos \theta, \quad (2.82)$$

$$c = \pm \frac{f(\mathbf{k})}{E_k \sqrt{2}} \sin \theta. \quad (2.83)$$

Using $E_k = \pm |f(\mathbf{k})|$ for the dispersive bands and introducing a phase factor via

$$f(\mathbf{k}) = e^{i\theta_{\mathbf{k}}} |f(\mathbf{k})|, \quad (2.84)$$

the normalized eigenstates $|\psi_{\pm}\rangle$ corresponding to the conduction (+) and valence (−) bands can be written as

$$|\psi_{\pm}\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} \cos \theta e^{i\theta_{\mathbf{k}}} \\ \pm 1 \\ \sin \theta e^{-i\theta_{\mathbf{k}}} \end{pmatrix}, \quad (2.85)$$

where the upper and lower signs correspond to the conduction and valence bands, respectively.

We now determine the eigenket associated with the flat band, characterized by $E_{\mathbf{k}} = 0$. In this case, the coefficients of the eigenvector must satisfy the following system of equations:

$$bf(\mathbf{k}) \cos \theta = 0, \quad (2.86)$$

$$af^*(\mathbf{k}) \cos \theta + cf(\mathbf{k}) \sin \theta = 0, \quad (2.87)$$

$$bf^*(\mathbf{k}) \sin \theta = 0. \quad (2.88)$$

From Eqs. (2.86)–(2.88), we immediately conclude that $b = 0$. The normalization condition for the ket then reduces to

$$|a|^2 + |c|^2 = 1. \quad (2.89)$$

Solving Eq. (2.87) for a and subsequently multiplying by its complex conjugate, we obtain

$$|a|^2 = |c|^2 \tan^2 \theta. \quad (2.90)$$

Substituting this result into the normalization condition (2.89) and choosing an appropriate global phase, we may write

$$c = -\cos \theta, \quad a = \frac{f(\mathbf{k})}{f^*(\mathbf{k})} \sin \theta. \quad (2.91)$$

Since the overall phase of a ket is arbitrary, it is convenient to express the state in terms of a phase factor $e^{-i\theta_{\mathbf{k}}}$, yielding

$$c = -\cos \theta e^{-i\theta_{\mathbf{k}}}, \quad a = \sin \theta e^{i\theta_{\mathbf{k}}}. \quad (2.92)$$

Consequently, the normalized eigenket corresponding to the flat band can be written as

$$|\psi_0\rangle = \begin{pmatrix} \sin \theta e^{i\theta_{\mathbf{k}}} \\ 0 \\ -\cos \theta e^{-i\theta_{\mathbf{k}}} \end{pmatrix}. \quad (2.93)$$

Having obtained the eigenfunctions, one can, in principle, analyze the transmission of fermionic quasiparticles in the $\alpha - T_3$ lattice through electrostatic potential barriers, thereby enabling a detailed study of Klein and super-Klein tunneling phenomena. These transport properties, however, lie beyond the scope of this master's thesis. For comprehensive discussions of such effects in the $\alpha - T_3$ model, we refer the reader to Refs. (URBAN *et al.*, 2011; ILLES; NICOL, 2017a; BETANCUR-OCAMPO *et al.*, 2017; YE *et al.*, 2020).

3 TIGHT-BINDING HAMILTONIAN OF $\alpha - T_3$ NANORIBBONS

In the previous chapter, we examined the crystallographic properties of the $\alpha - T_3$ lattice and introduced the tight-binding formalism to describe its electronic properties in the infinite-system limit. In this chapter, we extend this analysis to investigate electronic properties under quantum confinement in a single spatial direction, focusing on $\alpha - T_3$ nanoribbons.

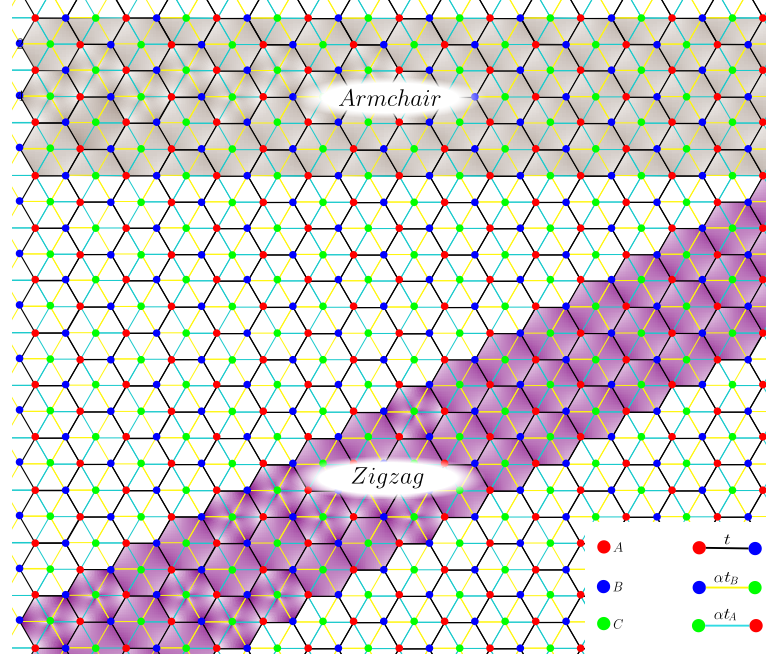
Nanoribbons derived from atomically thin lamellar crystals, composed of one or a few atomic layers, constitute a novel class of quasi-one-dimensional (1D) nanoscale materials (YAGMURCUKARDES *et al.*, 2016). Within the context of two-dimensional (2D) materials, nanoribbons are defined such that translational symmetry and periodicity are preserved along one direction, whereas in the transverse direction, only the atomic geometry is maintained, leading to a finite width and thus quantum confinement. This lateral confinement of charge carriers gives rise to a series of distinctive electronic features. A paradigmatic example is provided by graphene nanoribbons with armchair-type edge terminations, for which an energy gap emerges as a function of the ribbon width (WAKABAYASHI *et al.*, 2010; SHINDE *et al.*, 2022; SENA *et al.*, 2012).

Given that the $\alpha - T_3$ lattice includes graphene as one of its limiting cases, the objective of this chapter is to perform a systematic tight-binding study of $\alpha - T_3$ nanoribbons, with particular emphasis on the role of morphology. We will address limiting and intermediate (transition) regimes, as well as the distinct ways in which the central site is connected to the underlying honeycomb lattice, and analyze how these structural characteristics influence the resulting electronic properties. The $\alpha - T_3$ nanoribbons, analogous to graphene nanoribbons, exhibit edge terminations of the armchair and zigzag types, as illustrated in Fig. 20.

3.1 Tight-binding method for $\alpha - T_3$ nanoribbons

The $\alpha - T_3$ lattice is a crystal structure comprising three inequivalent sublattice sites, denoted by A , B , and C , as illustrated in Fig. 20. Within the nearest-neighbor tight-binding (TB) approximation for $\alpha - T_3$ nanoribbon, the Hamiltonian can be written

Figure 20 – Armchair and zigzag $\alpha - T_3$ nanoribbons. The A and B sites are connected via hopping energy t , and A and C (B and C) sites given by αt_A (αt_B), where α is a morphological parameter which allows interpolation between Graphene ($\alpha = 0$) and Dice ($\alpha = 1$) lattices.



Source: The author.

as

$$\hat{H} = \sum_i \epsilon_i \hat{n}_i + \sum_{i \neq j} t_{ij} \hat{g}_i^\dagger \hat{g}_j + \text{h.c.}, \quad (3.1)$$

which can be decomposed as

$$\hat{H} \equiv \underbrace{\hat{H}_o}_{\text{on-site}} + \underbrace{\hat{H}_h}_{\text{hopping}}. \quad (3.2)$$

For the $\alpha - T_3$ lattice, these contributions take the form

$$\hat{H}_o = \sum_i \epsilon_i^A \hat{a}_i^\dagger \hat{a}_i + \sum_i \epsilon_i^B \hat{b}_i^\dagger \hat{b}_i + \sum_i \epsilon_i^C \hat{c}_i^\dagger \hat{c}_i, \quad (3.3)$$

$$\hat{H}_h = t \sum_{i \neq j} \left(\hat{a}_i^\dagger \hat{b}_j + \hat{b}_j^\dagger \hat{a}_i \right) + \alpha t_A \sum_{i \neq j} \left(\hat{a}_i^\dagger \hat{c}_j + \hat{c}_j^\dagger \hat{a}_i \right) + \alpha t_B \sum_{i \neq j} \left(\hat{b}_i^\dagger \hat{c}_j + \hat{c}_j^\dagger \hat{b}_i \right), \quad (3.4)$$

where t , αt_A , and αt_B denote the hopping amplitudes associated with the $A-B$, $A-C$, and $B-C$ bonds, respectively. The remaining quantities are defined as follows:

- ϵ_i is the on-site energy at site $i = A, B, C$;
- $\hat{n}_i = \hat{g}_i^\dagger \hat{g}_i$ is the number operator, which yields the electron occupation at the i th atomic site;
- $\hat{g}_i^\dagger$ ($\hat{g}_i$) creates (annihilates) an electron or a hole at the i th atomic site.

We now consider zigzag and armchair nanoribbons that are translationally invariant along the x -direction, while being finite along the y -direction, where their width is determined by the number of atomic lines. In other words, the $\alpha - T_3$ nanoribbon extends infinitely along the x -axis and has a finite size along the y -axis. Consequently, it is convenient to express the creation and annihilation operators in a Fourier basis along the x -direction and work in momentum space. Thus, we write

$$\hat{g}_i = \frac{1}{\sqrt{N}} \sum_{k_x} \sum_{n=1}^N e^{ik_x x_i} \hat{g}_{k_x, n}, \quad (3.5)$$

$$\hat{g}_i^\dagger = \frac{1}{\sqrt{N}} \sum_{k_x} \sum_{n=1}^N e^{-ik_x x_i} \hat{g}_{k_x, n}^\dagger, \quad (3.6)$$

where N is the number of unit cells, $g \in \{a, b, c\}$, and $\hat{g}_i$ annihilates (creates) an electron with momentum component $\hbar k_x$ at a site of type g belonging to line n .

We first consider the on-site energy contribution to the Hamiltonian. For the A sublattice, using Eqs. (3.5) and (3.6), we obtain

$$\sum_i \epsilon_A \hat{a}_i^\dagger \hat{a}_i = \sum_i \sum_{k_x, k'_x} \sum_{n, n'} \epsilon_A e^{-i(k'_x - k_x)x_i} \hat{a}_{k_x, n}^\dagger \hat{a}_{k'_x, n'}, \quad (3.7)$$

which, after interchanging the order of summations and employing

$$\frac{1}{N} \sum_i e^{-i(k'_x - k_x)x_i} = \delta_{k_x, k'_x}, \quad (3.8)$$

reduces to

$$\sum_i \epsilon_A \hat{a}_i^\dagger \hat{a}_i = \sum_{k_x} \sum_{n, n'} \epsilon_A \hat{a}_{k_x, n}^\dagger \hat{a}_{k_x, n'}. \quad (3.9)$$

Proceeding analogously for the B and C sublattices, we obtain

$$\sum_i \epsilon_B \hat{b}_i^\dagger \hat{b}_i = \sum_{k_x} \sum_{n, n'} \epsilon_B \hat{b}_{k_x, n}^\dagger \hat{b}_{k_x, n'}, \quad (3.10)$$

$$\sum_i \epsilon_C \hat{c}_i^\dagger \hat{c}_i = \sum_{k_x} \sum_{n, n'} \epsilon_C \hat{c}_{k_x, n}^\dagger \hat{c}_{k_x, n'}. \quad (3.11)$$

Therefore, the total on-site contribution to the Hamiltonian can be written as

$$\hat{H}_0 = \sum_{k_x} \sum_{n, n'} \epsilon_A \hat{a}_{k_x, n}^\dagger \hat{a}_{k_x, n'} + \sum_{k_x} \sum_{n, n'} \epsilon_B \hat{b}_{k_x, n}^\dagger \hat{b}_{k_x, n'} + \sum_{k_x} \sum_{n, n'} \epsilon_C \hat{c}_{k_x, n}^\dagger \hat{c}_{k_x, n'}. \quad (3.12)$$

For the Hamiltonian H_h , we first perform the rescaling $\cos \theta H_h$ and define the parameter $\alpha = \tan \theta$. Using Eqs. (3.5) and (3.6), the rescaled Hamiltonian¹ restricted to the $\hat{g}_i^\dagger \hat{d}_j$ terms can be written as

$$\begin{aligned} \hat{H}_\theta = & \frac{t \cos \theta}{\sqrt{N}} \sum_{i \neq j} \sum_{k_x, k'_x} \sum_{n, n'} e^{-ik_x x_i} e^{ik'_x x_j} \hat{a}_{k_x, n}^\dagger \hat{b}_{k'_x, n'} \\ & + \frac{t_A \sin \theta}{\sqrt{N}} \sum_{i \neq j} \sum_{k_x, k'_x} \sum_{n, n'} e^{-ik_x x_i} e^{ik'_x x_j} \hat{a}_{k_x, n}^\dagger \hat{c}_{k'_x, n'} \\ & + \frac{t_B \sin \theta}{\sqrt{N}} \sum_{i \neq j} \sum_{k_x, k'_x} \sum_{n, n'} e^{-ik_x x_i} e^{ik'_x x_j} \hat{b}_{k_x, n}^\dagger \hat{c}_{k'_x, n'}. \end{aligned} \quad (3.13)$$

By substituting $x_j = -(x_i - x_j) + x_i$ and regrouping like terms, Eq. (3.13) can be recast as

$$\begin{aligned} \hat{H}_\theta = & t \cos \theta \sum_{k_x, k'_x} \sum_{n, n'} \sum_i \frac{e^{-i(k'_x - k_x)x_i}}{N} \sum_j e^{-ik'_x(x_i - x_j)} \hat{a}_{k_x, n}^\dagger \hat{b}_{k'_x, n'} \\ & + t_A \sin \theta \sum_{k_x, k'_x} \sum_{n, n'} \sum_i \frac{e^{-i(k'_x - k_x)x_i}}{N} \sum_j e^{-ik'_x(x_i - x_j)} \hat{a}_{k_x, n}^\dagger \hat{c}_{k'_x, n'} \\ & + t_B \sin \theta \sum_{k_x, k'_x} \sum_{n, n'} \sum_i \frac{e^{-i(k'_x - k_x)x_i}}{N} \sum_j e^{-ik'_x(x_i - x_j)} \hat{b}_{k_x, n}^\dagger \hat{c}_{k'_x, n'}, \end{aligned} \quad (3.14)$$

where the index i is held fixed while performing the summation over j . Using Eq. (3.8), Eq. (3.14) then takes the form

$$\begin{aligned} \hat{H}_\theta = & \sum_{k_x, n, n'} \tau_{n, n'}^{AB}(k_x) \hat{a}_{k_x, n}^\dagger \hat{b}_{k_x, n'} + \sum_{k_x, n, n'} \tau_{n, n'}^{BA}(k_x) \hat{b}_{k_x, n}^\dagger \hat{a}_{k_x, n'} \\ & + \sum_{k_x, n, n'} \tau_{n, n'}^{AC}(k_x) \hat{a}_{k_x, n}^\dagger \hat{c}_{k_x, n'} + \sum_{k_x, n, n'} \tau_{n, n'}^{CA}(k_x) \hat{c}_{k_x, n}^\dagger \hat{a}_{k_x, n'} \\ & + \sum_{k_x, n, n'} \tau_{n, n'}^{BC}(k_x) \hat{b}_{k_x, n}^\dagger \hat{c}_{k_x, n'} + \sum_{k_x, n, n'} \tau_{n, n'}^{CB}(k_x) \hat{c}_{k_x, n}^\dagger \hat{b}_{k_x, n'}, \end{aligned} \quad (3.15)$$

where the hopping amplitudes satisfy

$$(\tau_{n, n'}^{AB}(k_x))^* = \tau_{n, n'}^{BA}(k_x) = t \cos \theta \sum_j e^{i\mathbf{K} \cdot \mathbf{R}_{ABj}}, \quad (3.16)$$

$$(\tau_{n, n'}^{AC}(k_x))^* = \tau_{n, n'}^{CA}(k_x) = t \sin \theta \sum_j e^{i\mathbf{K} \cdot \mathbf{R}_{ACj}} \quad (3.17)$$

$$(\tau_{n, n'}^{BC}(k_x))^* = \tau_{n, n'}^{CB}(k_x) = t \sin \theta \sum_j e^{i\mathbf{K} \cdot \mathbf{R}_{BCj}}, \quad (3.18)$$

¹ As discussed in Chapter 2, the morphological factor of the $\alpha - T_3$ lattice appears solely as an overall multiplicative factor multiplying a graphene-like band structure. This observation motivates adopting a normalized representation.

with $\mathbf{K} = (k_x, 0)$, $\mathbf{R}_{AB_j} = \mathbf{R}_A - \mathbf{R}_{B_j}$, and analogous definitions for the other pairs. Here, $\mathbf{R}$ denotes the lattice-site position vector. The corresponding band structure is then obtained by solving the Heisenberg equations of motion for the annihilation and creation operators.

3.2 Band structure of $\alpha - T_3$ nanoribbons

The Heisenberg equation of motion for the annihilation (creation) operators in Fourier space is given by

$$i\hbar \frac{d\hat{g}_{k_x,n}}{dt} = [\hat{g}_{k_x,n}, \hat{H}_\theta] = E_\theta \hat{g}_{k_x,n}, \quad (3.19)$$

where $g = \{a, b, c\}$, and we have assumed a temporal dependence of the form $\exp[-iE_\theta t/\hbar]$ for the modes², with E_θ denoting the rescaled energy spectrum. Since electrons are fermionic particles, the corresponding operators satisfy the canonical anticommutation relations

$$\{\hat{g}_{k_x,n}, \hat{g}_{k'_x,n'}^\dagger\} = \delta_{k_x,k'_x} \delta_{n,n'}; \quad (3.20a)$$

$$\{\hat{g}_{k_x,n}, \hat{g}_{k'_x,n'}\} = \{\hat{g}_{k_x,n}^\dagger, \hat{g}_{k'_x,n'}^\dagger\} = 0; \quad (3.20b)$$

$$\{\hat{g}_{k_x,n}, \hat{d}_{k'_x,n'}^\dagger\} = 0; \quad (3.20c)$$

$$\{\hat{g}_{k_x,n}, \hat{d}_{k'_x,n'}\} = \{\hat{g}_{k_x,n}^\dagger, \hat{d}_{k'_x,n'}^\dagger\} = 0, \quad (3.20d)$$

where $g \neq d$. Furthermore, for products of fermionic operators, we use

$$[\hat{g}, \hat{d}\hat{f}] = \{\hat{g}, \hat{d}\}\hat{f} - \hat{d}\{\hat{g}, \hat{f}\}. \quad (3.21)$$

Based on these anticommutation relations and the Heisenberg equation, we can determine the energy spectrum of the nanoribbons. To this end, we evaluate the commutators $[\hat{g}_{k_x,n}, \hat{H}]$, where the total Hamiltonian is decomposed as $\hat{H} = \hat{H}_0 + \hat{H}_\theta$.

² This assumption, $\hat{g}_{k_x,n}(t) = \hat{g}_{k_x,n} e^{-iE_\theta t/\hbar}$, is fully justified: the Hamiltonian $\hat{H}$ is time-independent and couples modes only through terms of the form $\hat{g}_{k_x,n}^\dagger \hat{g}_{k'_x,n'}$. As a result, the operator's time evolution boils down to a simple phase factor—no additional time dependence appears.

Using Eqs. (3.12), (3.15), and (3.21), we obtain

$$\begin{aligned}
[\hat{a}_{k_x, n}, \hat{H}] = & \sum_{k'_x, n, n'} \epsilon_i^A [\hat{a}_{k_x, n}, \hat{a}_{k'_x, n}^\dagger \hat{a}_{k'_x, n'}] \xrightarrow{\hat{a} \delta_{k_x, k'_x} \delta_{n, n'}} + \sum_{k'_x, n, n'} \tau_{n, n'}^{AB} [\hat{a}_{k_x, n}, \hat{a}_{k'_x, n}^\dagger \hat{b}_{k'_x, n'}] \xrightarrow{\hat{b} \delta_{k_x, k'_x} \delta_{n, n'}} \\
& + \sum_{k'_x, n, n'} \tau_{n, n'}^{BA} [\hat{a}_{k_x, n}, \hat{b}_{k'_x, n}^\dagger \hat{a}_{k'_x, n'}] \xrightarrow{0} + \sum_{k'_x, n, n'} \tau_{n, n'}^{AC} [\hat{a}_{k_x, n}, \hat{a}_{k'_x, n}^\dagger \hat{c}_{k'_x, n'}] \xrightarrow{\hat{c} \delta_{k_x, k'_x} \delta_{n, n'}} \\
& + \sum_{k'_x, n, n'} \tau_{n, n'}^{CA} [\hat{a}_{k_x, n}, \hat{c}_{k'_x, n}^\dagger \hat{a}_{k'_x, n'}] \xrightarrow{0} + \sum_{k'_x, n, n'} \tau_{n, n'}^{BC} [\hat{a}_{k_x, n}, \hat{b}_{k'_x, n}^\dagger \hat{c}_{k'_x, n'}] \xrightarrow{0} \\
& + \sum_{k'_x, n, n'} \tau_{n, n'}^{CB} [\hat{a}_{k_x, n}, \hat{c}_{k'_x, n}^\dagger \hat{b}_{k'_x, n'}] \xrightarrow{0}, \tag{3.22}
\end{aligned}$$

and, by comparison with Eq. (3.19), this yields

$$\begin{aligned}
[\hat{a}_{k_x, n}, \hat{H}] = & \sum_{n'} \epsilon_i^A \hat{a}_{k_x, n'} + \sum_{n'} \tau_{n'}^{AB}(k_x) \hat{b}_{k_x, n'} \\
& + \sum_{n'} \tau_{n'}^{AC}(k_x) \hat{c}_{k_x, n'} = E \hat{a}_{k_x, n}, \quad n = 1, 2, 3, \dots, N_A. \tag{3.23}
\end{aligned}$$

Performing the same procedure for the remaining operators, we obtain

$$\begin{aligned}
[\hat{b}_{k_x, n}, \hat{H}] = & \sum_{n'} \epsilon_i^B \hat{b}_{k_x, n'} + \sum_{n'} \tau_{n'}^{BA}(k_x) \hat{a}_{k_x, n'} \\
& + \sum_{n'} \tau_{n'}^{BC}(k_x) \hat{c}_{k_x, n'} = E \hat{b}_{k_x, n}, \quad n = 1, 2, 3, \dots, N_B, \tag{3.24}
\end{aligned}$$

$$\begin{aligned}
[\hat{c}_{k_x, n}, \hat{H}] = & \sum_{n'} \epsilon_i^C \hat{c}_{k_x, n'} + \sum_{n'} \tau_{n'}^{CA}(k_x) \hat{a}_{k_x, n'} \\
& + \sum_{n'} \tau_{n'}^{CB}(k_x) \hat{b}_{k_x, n'} = E \hat{c}_{k_x, n}, \quad n = 1, 2, 3, \dots, N_C. \tag{3.25}
\end{aligned}$$

These equations can be written compactly in matrix form as

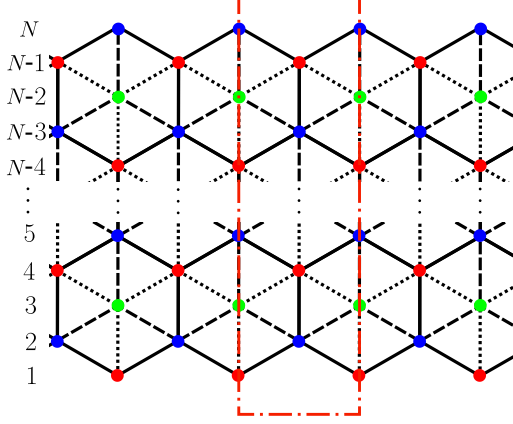
$$T(k_x) \begin{pmatrix} \hat{a}_{k_x, n} \\ \hat{b}_{k_x, n} \\ \hat{c}_{k_x, n} \end{pmatrix} = E \begin{pmatrix} \hat{a}_{k_x, n} \\ \hat{b}_{k_x, n} \\ \hat{c}_{k_x, n} \end{pmatrix}, \tag{3.26}$$

where $T(k_x)$ is a matrix of dimension $(N_A + N_B + N_C) \times (N_A + N_B + N_C)$. Its block structure can be represented as

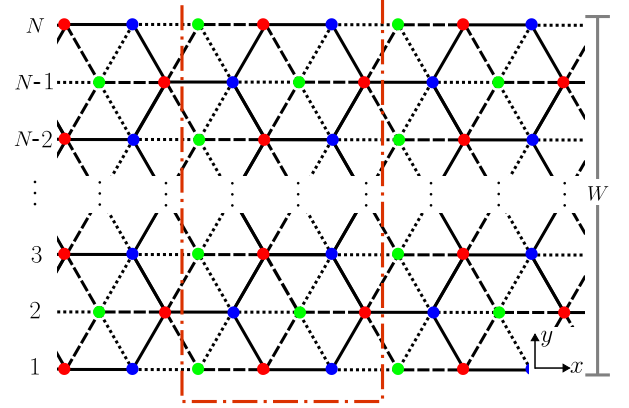
$$T(k_x) = \begin{pmatrix} [\epsilon^A]_{N_A \times N_A} & [\tau^{AB}]_{N_A \times N_B} & [\tau^{AC}]_{N_A \times N_C} \\ [\tau^{BA}]_{N_B \times N_A} & [\epsilon^B]_{N_B \times N_B} & [\tau^{BC}]_{N_B \times N_C} \\ [\tau^{CA}]_{N_C \times N_A} & [\tau^{CB}]_{N_C \times N_B} & [\epsilon^C]_{N_C \times N_C} \end{pmatrix}, \tag{3.27}$$

Figure 21 – The rectangle delimited by the dashed line denotes the unit cell. The nanoribbon width W is defined by specifying the number of atomic chains across the transverse direction.

(a) Zigzag $\alpha - T_3$ nanoribbon.



(b) Armchair $\alpha - T_3$ nanoribbon.



Source: The author.

where $[\epsilon^i]_{N_i \times N_i}$ is a diagonal (or, in the simplest case, null) matrix of dimension $N_i \times N_i$, containing the on-site energies for sublattice $i \in \{A, B, C\}$. Since our tight-binding model includes only first-nearest-neighbor interactions, the matrix elements of the hopping blocks $[\tau]_{N_i \times N_j}$ can be considerably simplified for the specific geometries corresponding to zigzag and armchair nanoribbon edges.

The schematic representations of nanoribbons with zigzag and armchair terminations in the $\alpha - T_3$ lattice are shown below.

3.3 Zigzag case

In the case of $Z\alpha - T_3$ NRs under the nearest-neighbor approximation, the matrix elements τ^{AB} , τ^{AC} , and τ^{BC} defined in (3.18) take the general form

$$\tau_{n,n'}^{AB} = \gamma^{AB}(t) \delta_{n_a, n_b+2} + \eta^{AB}(t) \delta_{n_a, n_b-1}, \quad (3.28a)$$

$$\tau_{n,n'}^{AC} = \gamma^{AC}(t_A) \delta_{n_a, n_c+1} + \eta^{AC}(t_A) \delta_{n_a, n_c-2}, \quad (3.28b)$$

$$\tau_{n,n'}^{BC} = \gamma^{BC}(t_B) \delta_{n_b, n_c+2} + \eta^{BC}(t_B) \delta_{n_b, n_c-1}, \quad (3.28c)$$

where n_j ($j = a, b, c$) denotes the position of each nonequivalent site in terms of the nanoribbon index. Specifically, one has $n_a = 1, 4, 7, \dots, N_A$, $n_b = 2, 5, 8, \dots, N_B$, and $n_c = 3, 6, 9, \dots, N_C$.

By analyzing the nanoribbon geometry, we can explicitly determine the coefficients $\gamma^{(\dots)}$ and $\eta^{(\dots)}$. Consider first the term $\tau_{n_a, n_b'}^{AB}$. For $n_a = 1$ we obtain $\delta_{n_a, n_b+2} = 0$ for

all n_b , whereas $\delta_{n_a, n_b-1} = 1$ for $n_b = 2$. Consequently,

$$\tau_{n_a=1, n_b=2}^{AB} = \eta^{AB} = t \cos \theta (e^{i\mathbf{k} \cdot \mathbf{d}_2} + e^{i\mathbf{k} \cdot \mathbf{d}_3}), \quad (3.29)$$

where $\mathbf{k} = (k_x \ 0)^T$ and the lattice vectors are given by $\mathbf{d}_1 = (0 \ 1)^T a$, $\mathbf{d}_2 = (-\sqrt{3} \ -1)^T a/2$, and $\mathbf{d}_3 = (\sqrt{3} \ -1)^T a/2$. Next, for $n_a = 4$ we have $\delta_{n_a, n_b+2} = 1$ for $n_b = 2$ and $\delta_{n_a, n_b-1} = 0$ for all n_b , thus

$$\tau_{n_a=4, n_b=2}^{AB} = \gamma^{AB} = t \cos \theta e^{i\mathbf{k} \cdot \mathbf{d}_1}. \quad (3.30)$$

Since the lattice geometry is translationally invariant along the nanoribbon, the same reasoning applies to all other pairs of indices. Therefore, for any allowed combination of n_a and n_b , one finds $\gamma^{AB} = t \cos \theta e^{i\mathbf{k} \cdot \mathbf{d}_1}$, $\eta^{AB} = t \cos \theta (e^{i\mathbf{k} \cdot \mathbf{d}_2} + e^{i\mathbf{k} \cdot \mathbf{d}_3})$.

We now turn to the term $\tau_{n,n'}^{AC}$. For $n_a = 1$ we obtain $\delta_{n_a, n_c+1} = 0$ for all n_c , whereas $\delta_{n_a, n_c-2} = 1$ for $n_c = 3$. In this case,

$$\eta^{AC} = t_A \sin \theta e^{-i\mathbf{k} \cdot \mathbf{d}_1}. \quad (3.31)$$

For $n_a = 4$, $\delta_{n_a, n_c+1} = 1$ for $n_c = 3$, which yields

$$\gamma^{AC} = t_A \sin \theta (e^{-i\mathbf{k} \cdot \mathbf{d}_2} + e^{-i\mathbf{k} \cdot \mathbf{d}_3}). \quad (3.32)$$

Repeating this procedure for the remaining terms, the same expressions are obtained for all admissible combinations of n_a and n_c , namely $\gamma^{AC} = t_A \sin \theta (e^{-i\mathbf{k} \cdot \mathbf{d}_2} + e^{-i\mathbf{k} \cdot \mathbf{d}_3})$, $\eta^{AC} = t_A \sin \theta e^{-i\mathbf{k} \cdot \mathbf{d}_1}$. Finally, applying an analogous analysis to the term $\tau_{n,n'}^{BC}$, one obtains for all combinations of n_b and n_c : $\gamma^{BC} = t_B \sin \theta e^{i\mathbf{k} \cdot \mathbf{d}_1}$, $\eta^{BC} = t_B \sin \theta (e^{i\mathbf{k} \cdot \mathbf{d}_2} + e^{i\mathbf{k} \cdot \mathbf{d}_3})$.

We now analyze the zigzag-terminated edges of nanoribbons with arbitrary width in order to construct the corresponding tight-binding Hamiltonian. For a zigzag edge of type AA, the admissible ribbon widths are $W = 1, 4, 7, \dots$. For $W = 1$, the number of atomic chains (or atomic lines) of each sublattice type is $N_A = 1$ and $N_B = N_C = 0$. For $W = 2$, one finds $N_A = 2$, $N_B = 1$, and $N_C = 1$. Proceeding in this manner, one obtains the values summarized in Table 1.

Table 1 – Number of atomic lines of type N_i ($i = A, B, C$) for a zigzag termination of type AA as a function of the ribbon width W_{AA} .

W_{AA}	N_A	N_B	N_C
1	1	0	0
4	2	1	1
7	3	2	2
$\vdots$	$\vdots$	$\vdots$	$\vdots$
N	$\frac{N+2}{3}$	$\frac{N-1}{3}$	$\frac{N-1}{3}$

For the remaining zigzag terminations of the nanoribbon, the corresponding distributions of atomic lines are given in the following tables.

Table 2 – Number of atomic lines of type N_i ($i = A, B, C$) for a zigzag termination of type AB as a function of the ribbon width W_{AB} .

W_{AB}	N_A	N_B	N_C
2	1	1	0
5	2	2	1
8	3	3	2
$\vdots$	$\vdots$	$\vdots$	$\vdots$
N	$\frac{N+1}{3}$	$\frac{N+1}{3}$	$\frac{N-2}{3}$

Table 3 – Number of atomic lines of type N_i ($i = A, B, C$) for a zigzag termination of type AC as a function of the ribbon width W_{AC} .

W_{AC}	N_A	N_B	N_C
3	1	1	1
6	2	2	2
9	3	3	3
$\vdots$	$\vdots$	$\vdots$	$\vdots$
N	$\frac{N}{3}$	$\frac{N}{3}$	$\frac{N}{3}$

Consequently, for a zigzag edge the inter-sublattice hopping matrices $[\tau]_{N_i \times N_j}$ can be written explicitly as

$$[\tau]_{N_i \times N_j} = \begin{pmatrix} \eta^{ij} & 0 & 0 & \cdots & 0 \\ \gamma^{ij} & \eta^{ij} & 0 & \ddots & 0 \\ 0 & \gamma^{ij} & \eta^{ij} & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & 0 & \gamma^{ij} & \eta^{ij} \end{pmatrix}, \quad (3.33)$$

where $i \neq j = A, B, C$. The parameters η^{ij} and γ^{ij} that define the elements of the above matrices are organized and specified in the table below.

Table 4 – Element matrices for $Z\alpha - T_3$ NRs.

Element	Zigzag AA/AB/AC
$\gamma^{AB}(t)$	$t \cos \theta e^{i\mathbf{k} \cdot \mathbf{d}_1}$
$\eta^{AB}(t)$	$t \cos \theta (e^{i\mathbf{k} \cdot \mathbf{d}_2} + e^{i\mathbf{k} \cdot \mathbf{d}_3})$
$\gamma^{AC}(t_A)$	$t_A \sin \theta (e^{-i\mathbf{k} \cdot \mathbf{d}_2} + e^{-i\mathbf{k} \cdot \mathbf{d}_3})$
$\eta^{AC}(t_A)$	$t_A \sin \theta e^{-i\mathbf{k} \cdot \mathbf{d}_1}$
$\gamma^{BC}(t_B)$	$t_B \sin \theta e^{i\mathbf{k} \cdot \mathbf{d}_1}$
$\eta^{BC}(t_B)$	$t_B \sin \theta (e^{i\mathbf{k} \cdot \mathbf{d}_2} + e^{i\mathbf{k} \cdot \mathbf{d}_3})$

3.4 Armchair case

In the case of $A\alpha - T_3$ NRs under the first-nearest-neighbor approximation, the matrix elements τ^{AB} , τ^{AC} , and τ^{BC} defined in (3.18) take the general form

$$\tau_{n,n'}^{AB} = \gamma^{AB}(t) \delta_{n_a, n_b+1} + \eta^{AB}(t) \delta_{n_a, n_b} + \lambda^{AB}(t) \delta_{n_a, n_b-1}, \quad (3.34a)$$

$$\tau_{n,n'}^{AC} = \gamma^{AC}(t_A) \delta_{n_a, n_c+1} + \eta^{AC}(t_A) \delta_{n_a, n_c} + \lambda^{AC}(t_A) \delta_{n_a, n_c-1}, \quad (3.34b)$$

$$\tau_{n,n'}^{BC} = \gamma^{BC}(t_B) \delta_{n_b, n_c+1} + \eta^{BC}(t_B) \delta_{n_b, n_c} + \lambda^{BC}(t_B) \delta_{n_b, n_c-1}. \quad (3.34c)$$

These expressions give rise to the following tridiagonal coupling matrices:

$$[\tau]_{N_i \times N_j} = \begin{pmatrix} \eta^{ij} & \lambda^{ij} & 0 & \cdots & 0 \\ \gamma^{ij} & \eta^{ij} & \lambda^{ij} & \ddots & 0 \\ 0 & \gamma^{ij} & \eta^{ij} & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & \lambda^{ij} \\ 0 & 0 & 0 & \gamma^{ij} & \eta^{ij} \end{pmatrix} \quad \text{with } i \neq j = A, B, C. \quad (3.35)$$

Following a procedure analogous to the zigzag case, we first consider the term τ_{n_a, n_b}^{AB} . For $n_a = 1$ and $n_b = 1$, the only nonvanishing contribution corresponds to η^{AB} , whose value is

$$\eta^{AB} = t \cos \theta e^{-i\mathbf{k} \cdot \mathbf{d}_2}. \quad (3.36)$$

For $n_a = 1$ and $n_b = 2$, the surviving term is λ^{AB} , yielding

$$\lambda^{AB} = t \cos \theta e^{-i\mathbf{k} \cdot \mathbf{d}_3}. \quad (3.37)$$

For $n_a = 2$ and $n_b = 1$, the relevant term is γ^{AB} , given by

$$\gamma^{AB} = t \cos \theta e^{-i\mathbf{k} \cdot \mathbf{d}_1}. \quad (3.38)$$

The coefficients γ^{AB} , η^{AB} , and λ^{AB} retain these forms for the remaining admissible index combinations.

The next set of elements is τ_{n_a, n_c}^{AC} . Proceeding as before, for $n_a = 1$ and $n_c = 1$ we obtain

$$\eta^{AC} = t_A \sin \theta e^{i\mathbf{k} \cdot \mathbf{d}_2}, \quad (3.39)$$

for $n_a = 1$ and $n_c = 2$ we find

$$\lambda^{AC} = t_A \sin \theta e^{i\mathbf{k} \cdot \mathbf{d}_1}, \quad (3.40)$$

and for $n_a = 2$ and $n_c = 1$ we obtain

$$\gamma^{AC} = t_A \sin \theta e^{i\mathbf{k} \cdot \mathbf{d}_3}. \quad (3.41)$$

By applying the same procedure, the corresponding expressions for the BC terms can be derived; they are analogous to the AB case, but modulated by $\sin \theta$ (with the appropriate hopping parameter).

For the $A\alpha-T_3$ NRs configuration, the width of the nanoribbon W is equal to the number of lines of each sublattice type. Specifically, if $W = X$, then $N_A = N_B = N_C = X$. All results for the elements of the matrices $[\tau]_{N_i \times N_j}$ in the $A\alpha-T_3$ NRs case are summarized in Table 5.

Table 5 – Element matrices for $A\alpha-T_3$ NRs.

Element	Armchair
$\gamma^{AB}(t)$	$t \cos \theta e^{-i\mathbf{k} \cdot \mathbf{d}_1}$
$\eta^{AB}(t)$	$t \cos \theta e^{-i\mathbf{k} \cdot \mathbf{d}_2}$
$\lambda^{AB}(t)$	$t \cos \theta e^{-i\mathbf{k} \cdot \mathbf{d}_3}$
$\gamma^{AC}(t_A)$	$t_A \sin \theta e^{i\mathbf{k} \cdot \mathbf{d}_3}$
$\eta^{AC}(t_A)$	$t_A \sin \theta e^{i\mathbf{k} \cdot \mathbf{d}_2}$
$\lambda^{AC}(t_A)$	$t_A \sin \theta e^{i\mathbf{k} \cdot \mathbf{d}_1}$
$\gamma^{BC}(t_B)$	$t_B \sin \theta e^{-i\mathbf{k} \cdot \mathbf{d}_1}$
$\eta^{BC}(t_B)$	$t_B \sin \theta e^{-i\mathbf{k} \cdot \mathbf{d}_2}$
$\lambda^{BC}(t_B)$	$t_B \sin \theta e^{-i\mathbf{k} \cdot \mathbf{d}_3}$

3.5 Synthesis of the results

It is possible to synthesize the results for both edge configurations (zigzag and armchair), since the matrices $[\tau]_{N_i \times N_j}$ that compose the Hamiltonian in Eq. (3.27) share the same general structure. Their constituent elements $\gamma, \eta, \lambda = \gamma^{AB}(t), \eta^{AB}(t), \lambda^{AB}(t), \gamma^{AC}(t_A), \eta^{AC}(t_A), \lambda^{AC}(t_A)$, and $\gamma^{BC}(t_B), \eta^{BC}(t_B), \lambda^{BC}(t_B)$ are summarized in Table 6.

Table 6 – Matrix elements for each type of nanoribbon edge.

Element	Zigzag $AA/AB/AC$	Armchair
$\gamma^{AB}(t)$	$t \cos \theta e^{i\mathbf{k} \cdot \mathbf{d}_1}$	$t \cos \theta e^{-i\mathbf{k} \cdot \mathbf{d}_1}$
$\eta^{AB}(t)$	$t \cos \theta (e^{i\mathbf{k} \cdot \mathbf{d}_2} + e^{i\mathbf{k} \cdot \mathbf{d}_3})$	$t \cos \theta e^{-i\mathbf{k} \cdot \mathbf{d}_2}$
$\lambda^{AB}(t)$	0	$t \cos \theta e^{-i\mathbf{k} \cdot \mathbf{d}_3}$
$\gamma^{AC}(t_A)$	$t_A \sin \theta (e^{-i\mathbf{k} \cdot \mathbf{d}_2} + e^{-i\mathbf{k} \cdot \mathbf{d}_3})$	$t_A \sin \theta e^{i\mathbf{k} \cdot \mathbf{d}_3}$
$\eta^{AC}(t_A)$	$t_A \sin \theta e^{-i\mathbf{k} \cdot \mathbf{d}_1}$	$t_A \sin \theta e^{i\mathbf{k} \cdot \mathbf{d}_2}$
$\lambda^{AC}(t_A)$	0	$t_A \sin \theta e^{i\mathbf{k} \cdot \mathbf{d}_1}$
$\gamma^{BC}(t_B)$	$t_B \sin \theta e^{i\mathbf{k} \cdot \mathbf{d}_1}$	$t_B \sin \theta e^{-i\mathbf{k} \cdot \mathbf{d}_1}$
$\eta^{BC}(t_B)$	$t_B \sin \theta (e^{i\mathbf{k} \cdot \mathbf{d}_2} + e^{i\mathbf{k} \cdot \mathbf{d}_3})$	$t_B \sin \theta e^{-i\mathbf{k} \cdot \mathbf{d}_2}$
$\lambda^{BC}(t_B)$	0	$t_B \sin \theta e^{-i\mathbf{k} \cdot \mathbf{d}_3}$

Table 7 – Number of atomic lines of type N_i ($i = A, B, C$) for each type of nanoribbon.

	Zigzag AA	Zigzag AB	Zigzag AC	Armchair
N_A	$(N + 2)/3$	$(N + 1)/3$	$N/3$	N
N_B	$(N - 1)/3$	$(N + 1)/3$	$N/3$	N
N_C	$(N - 1)/3$	$(N - 2)/3$	$N/3$	N

Having constructed the matrices that encode the connectivity between atomic sites for the two possible edge terminations of the nanoribbons, we can now solve Eq. (3.26) in order to obtain the dispersion relations.

3.5.1 Results for $Z\alpha - T_3NRs$

By diagonalizing the Hamiltonian (3.27) for the $Z\alpha - T_3NRs$ configuration, we obtain the dispersion relations for the two distinct types of coupling between the honeycomb lattice and the central site, shown in Figs. 22 and 23, respectively. The dispersion relations exhibit clear differences for nanoribbons with different bonding configurations. These differences arise exclusively from the finite-size confinement and the specific edge termination, since, as demonstrated in Chapter 2, in the case of the infinite lattice, both coupling schemes lead to identical band structures.

In the first configuration (Fig. 22), we investigate the coupling between the honeycomb sublattice site A and the central site C , considering morphological angles in the range $0 < \theta \leq \pi/4$. In this regime, the dispersion relation exhibits a periodic dependence on the ribbon width W (defined as the number of atomic chains across the ribbon). Three distinct families arise as a function of W , namely $W = 3p + 2$, $W = 3p$, and $W = 3p + 1$, with $p = 1, 2, 3, \dots$. Nanoribbons with $W = 3p + 2$ and $W = 3p$ display semiconducting behavior, whereas those with $W = 3p + 1$ exhibit metallic character.

In the second configuration (Fig. 23), the coupling occurs between the honeycomb sublattice site B and the central site C , again for morphological angles in the interval $0 < \theta \leq \pi/4$. In this case, the dispersion relation also displays a periodic dependence on the ribbon width, analogous to the previous configuration, yielding the same three families: $W = 3p + 2$, $W = 3p$, and $W = 3p + 1$ with $p = 1, 2, 3, \dots$. However, in contrast to the t_A -coupling case, all three families now exhibit semiconducting behavior. The corresponding energy gaps satisfy

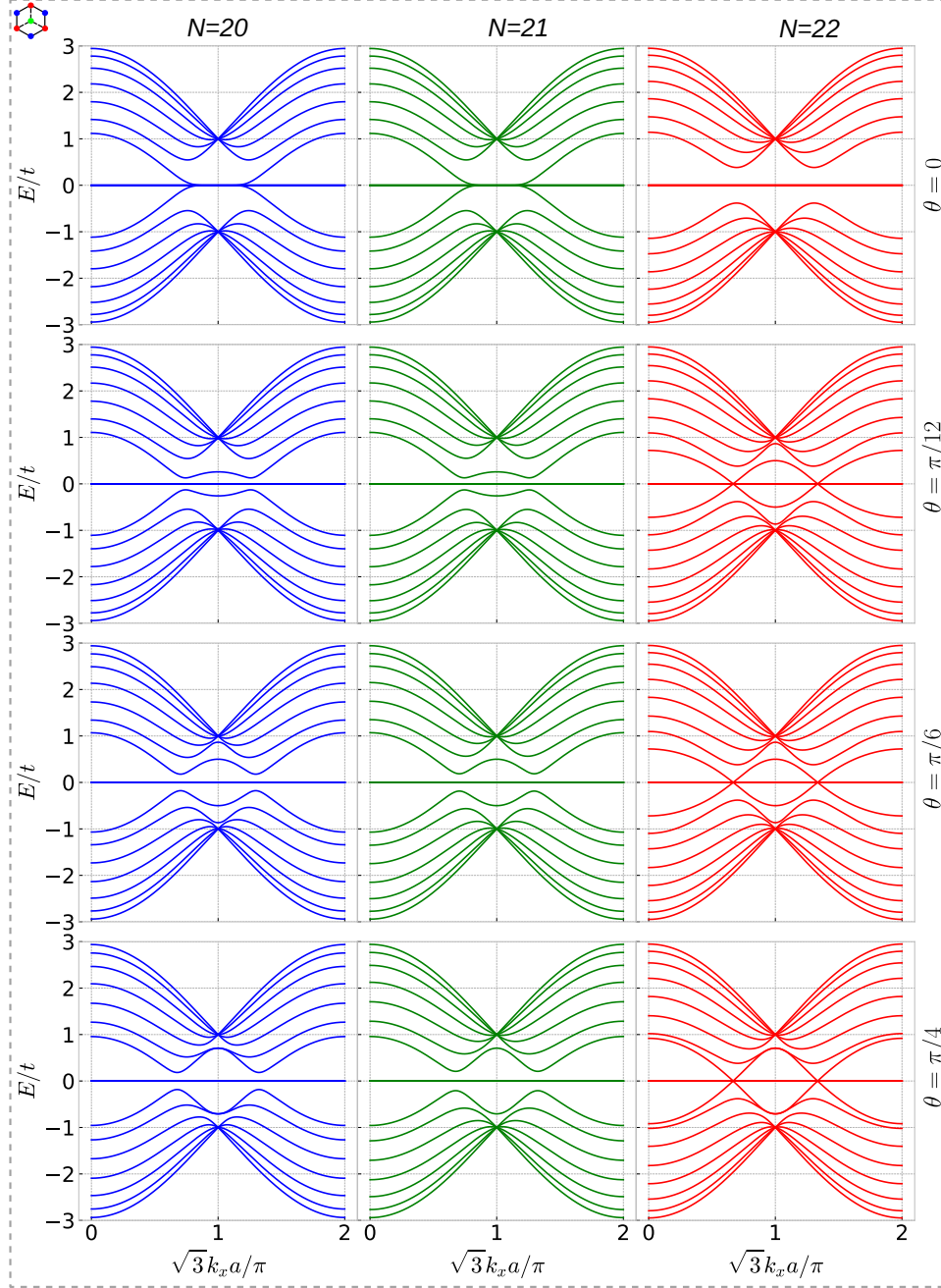
$$\text{gap}(3p + 1) > \text{gap}(3p) > \text{gap}(3p + 2), \quad (0 < \theta \leq \pi/4).$$

The special case $\theta = 0$ corresponds to the graphene limit. In this limit, the usual $3p$ classification does not hold, since graphene nanoribbons with zigzag edge termination are always metallic (WAKABAYASHI *et al.*, 2010). Nevertheless, for $N = 22$ and $\theta = 0$ we obtain a semiconducting nanoribbon. This behavior is a consequence of the underlying $\alpha - T_3$ model, which allows for three distinct types of edge termination, unlike graphene, whose unit cell contains only two inequivalent sites, giving rise to only two possible edge terminations. Tables 1, 2, and 3 summarize how the number of atomic lines is distributed among the inequivalent sites as a function of the ribbon width.

The energy gaps of the family of zigzag nanoribbons are always direct. Throughout this dissertation, we define the band gap as the difference between the minimum of the conduction band and the energy of the first state of the flat band³. In Fig. 24, we present the numerically obtained band gaps as a function of ribbon width for both coupling configurations discussed above. The results indicate that the band gap decreases with increasing ribbon width, approaching the behavior of the bulk (infinite) system, which is gapless; see Fig. 18.

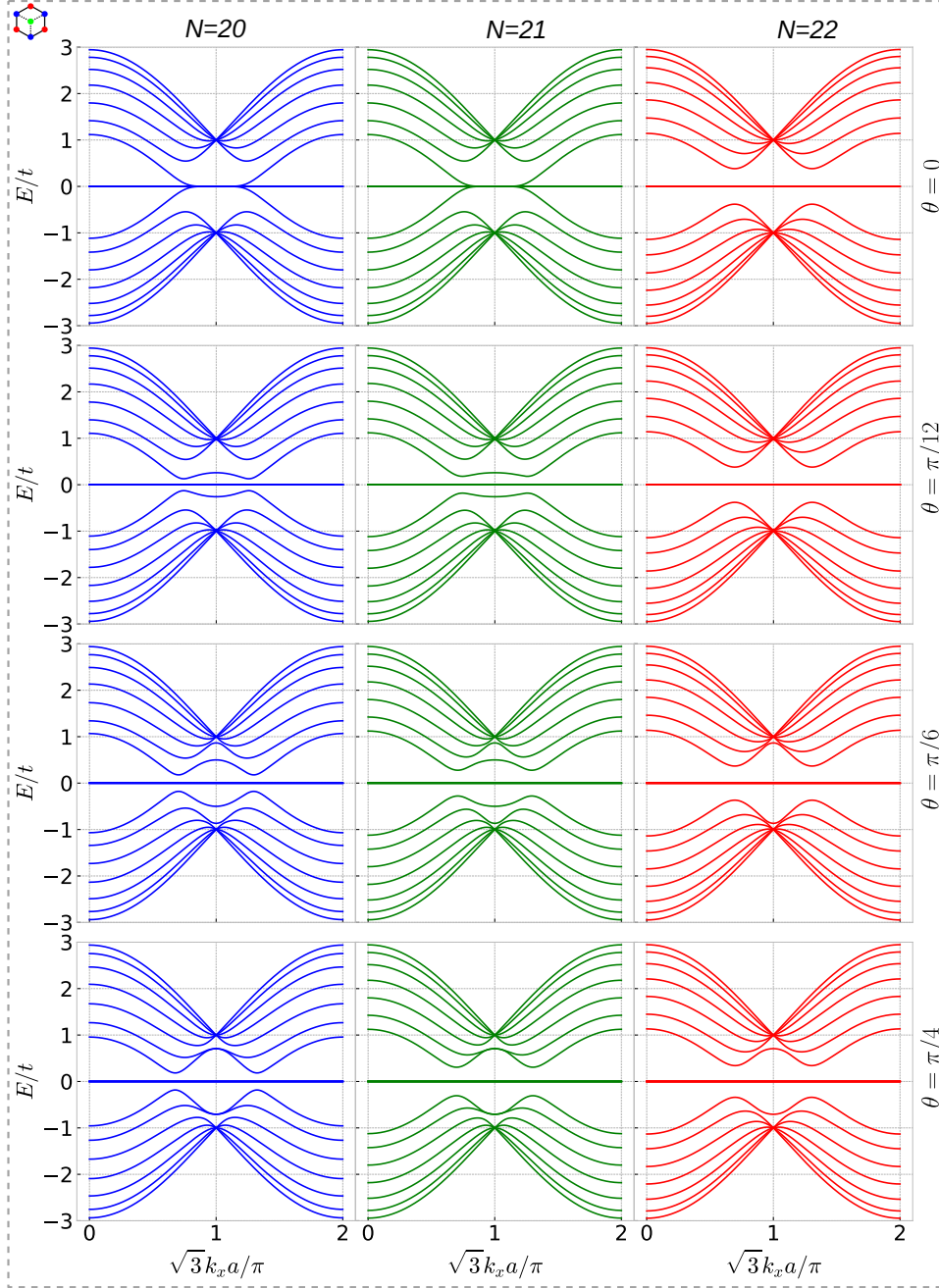
³ This definition of the energy gap as the minimum of the conduction band minus the flat band energy is convenient because the band structure of the $\alpha - T_3$ lattice possesses electron-hole symmetry.

Figure 22 – Band structures of zigzag $\alpha - T_3$ nanoribbons for $t_A = t$ and $t_B = 0$ with different edge terminations, ribbon widths, and morphological angle $\theta = \tan^{-1} \alpha$: $\theta = 0$, $\theta = \pi/12$, $\theta = \pi/6$, and $\theta = \pi/4$, for $N = 20$ (nanoribbon edge terminated by atomic line of type B), $N = 21$ (edge terminated by an atomic line of type C), and $N = 22$ (edge terminated by atomic line of type A).



Source: The author.

For the first coupling configuration ($t_A \neq 0$, $t_B = 0$), the families with $W = 3p$ and $W = 3p + 1$ are always semiconducting, while those with $W = 3p + 2$ are metallic. In contrast, for the second coupling configuration ($t_A = 0$, $t_B \neq 0$), all three families are semiconducting.

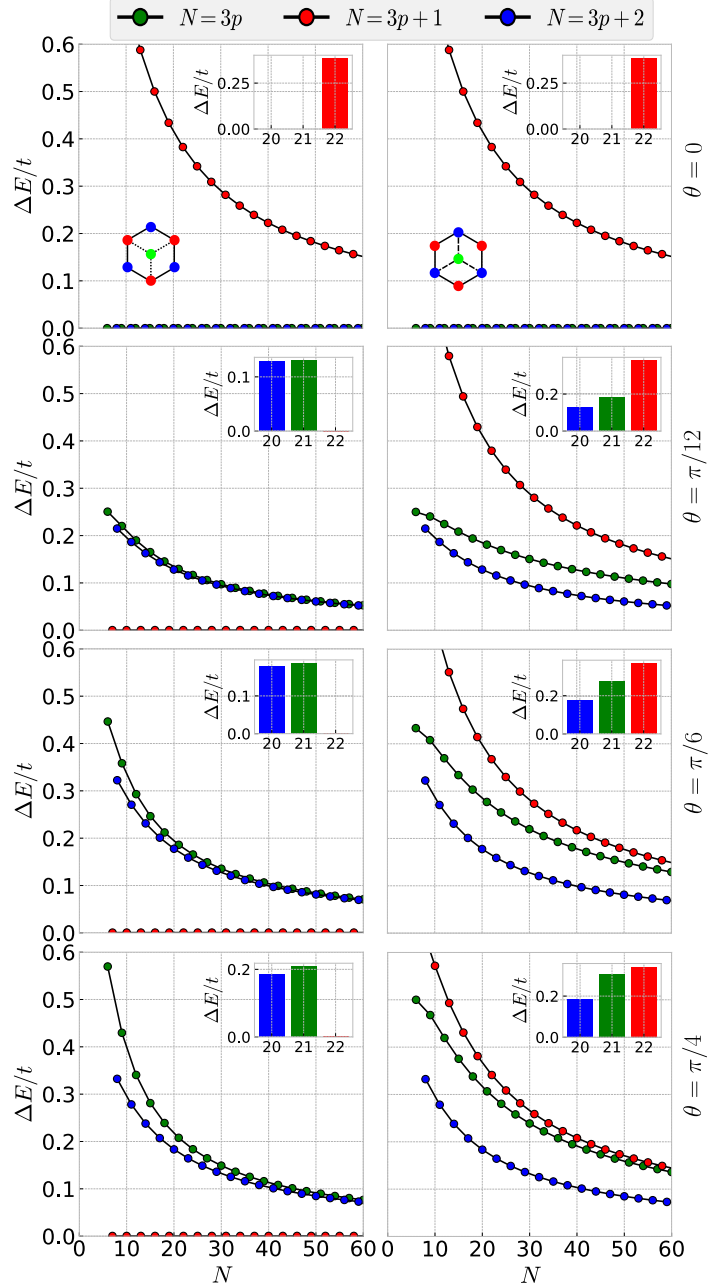
Figure 23 – Same as Fig. 22, but for $t_A = 0$ and $t_B = t$.

Source: The author.

3.5.2 Results for $A\alpha - T_3NRs$

By diagonalizing the Hamiltonian in Eq. (3.27) for the $A\alpha - T_3NRs$ nanoribbons, we obtain the corresponding dispersion relations considering the two distinct ways of connecting the honeycomb lattice to the central site. However, in contrast to the $Z\alpha - T_3NRs$ configuration, the dispersion relation for $A\alpha - T_3NRs$ does not depend either on the specific type of connection between the central and honeycomb sites or on the ribbon edge

Figure 24 – Energy gap of zigzag $\alpha - T_3$ nanoribbons as a function of the number of atomic lines. Left: coupling between the central site and the honeycomb site of type A ($t_A = t$, $t_B = 0$). Right: coupling between the central site and the honeycomb site of type B ($t_A = 0$, $t_B = t$). In both cases, we consider the morphological angles $\theta = 0, \pi/12, \pi/6$, and $\pi/4$.

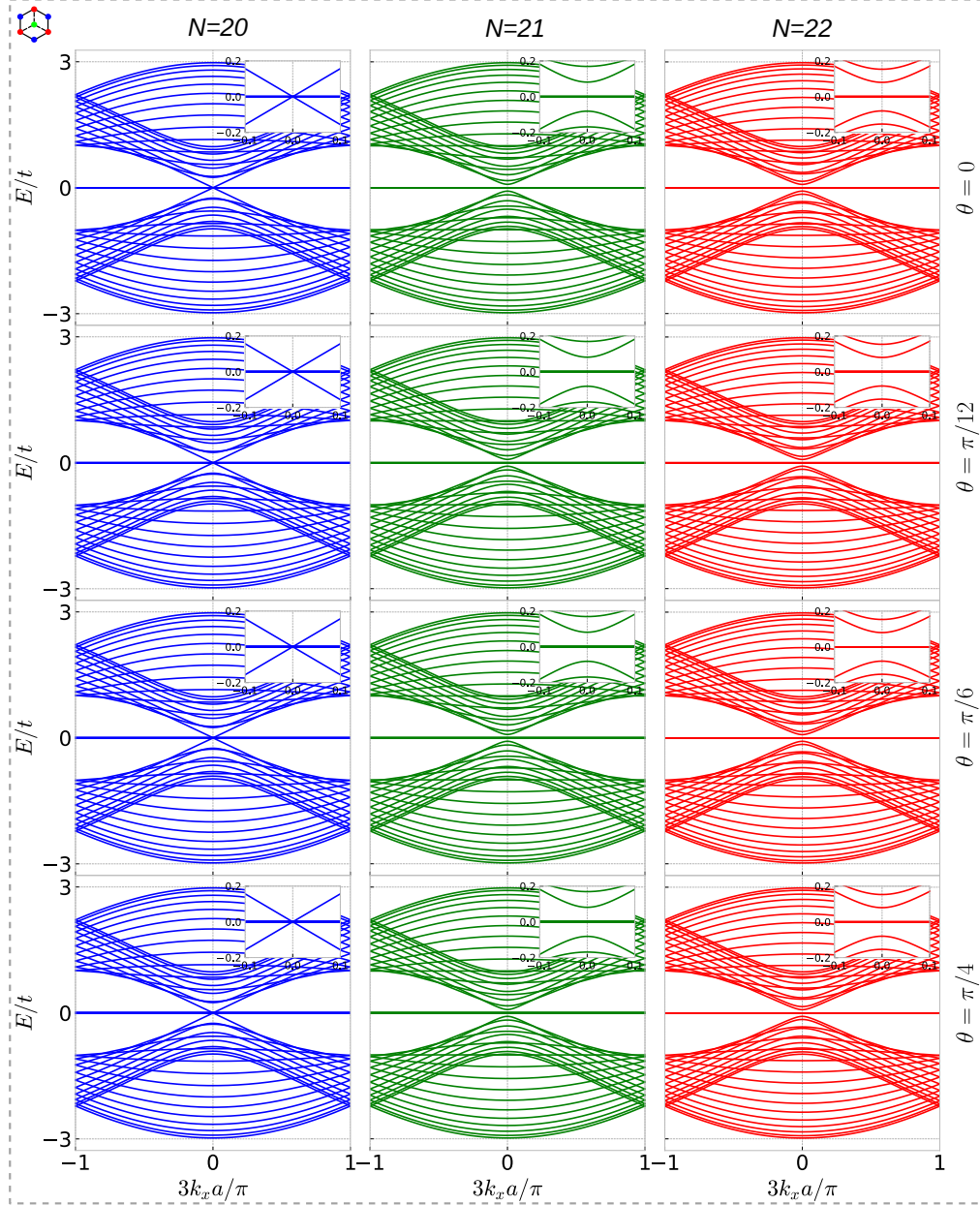


Source: The author.

morphology. Consequently, the band structures retain the same qualitative form as that shown in Fig. 25, where the dispersive bands coincide with those of graphene and only the flat band is absent.

An additional characteristic intrinsic to the $A\alpha - T_3$ NRs geometry is the strong dependence of its metallic or semiconducting character on the number of ribbon lines

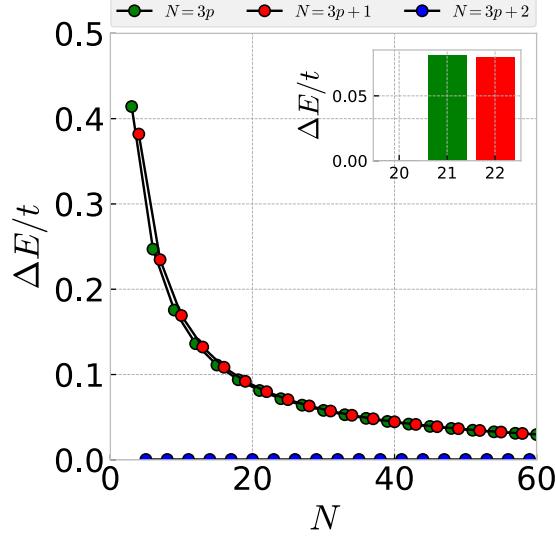
Figure 25 – Band structures for armchair $\alpha - T_3$ nanoribbons with different terminations, numbers of ribbon lines, and morphological angle $\theta = \tan^{-1} \alpha$: $\theta = 0$, $\theta = \pi/12$, $\theta = \pi/6$, and $\theta = \pi/4$.



Source: The author.

W . Analogously to armchair graphene nanoribbons, armchair $\alpha - T_3$ nanoribbons are semiconducting for $W = 3p$ and $W = 3p + 1$, and metallic for $W = 3p + 2$ ($p = 1, 2, 3, \dots$), as illustrated in Fig. 26.

Since the normalized dispersion relation of $A\alpha - T_3$ NRs coincides with that of graphene apart from the missing flat band, the dependence of the energy gap on the number of lines is also identical to that of armchair graphene nanoribbons. In the work by (SON *et al.*, 2006), an analytical expression was derived for the energy gap of the different

Figure 26 – Same as Fig.24 for $A\alpha - T_3$ NRs.

Source: The author.

armchair graphene nanoribbon families as a function of the number of lines, namely

$$\Delta E(p) = \begin{cases} t \left[4 \cos \left(\frac{p\pi}{3p+1} \right) - 2 \right], & N = 3p, \\ t \left[2 - 4 \cos \left(\frac{(p+1)\pi}{3p+2} \right) \right], & N = 3p+1, \\ 0, & N = 3p+2, \end{cases} \quad (3.42)$$

which can be equivalently written directly in terms of N as

$$\Delta E(N) = \begin{cases} t \left[4 \cos \left(\frac{\pi}{3} \frac{N}{N+1} \right) - 2 \right], & N = 3p, \\ t \left[2 - 4 \cos \left(\frac{\pi}{3} \frac{N+2}{N+1} \right) \right], & N = 3p+1, \\ 0, & N = 3p+2. \end{cases} \quad (3.43)$$

In the limit $N \rightarrow \infty$, we obtain $\Delta E(N) \rightarrow 0$, indicating that the system approaches an infinite lattice with a vanishing energy gap. Figure 26 shows the numerically calculated energy gap as a function of the number of ribbon lines for $A\alpha - T_3$ NRs, which is in exact agreement with the analytical prediction given by Eq. (3.42). In the limit of a large number of lines, the energy gap vanishes, as expected, and the gap satisfies the following relations: $\text{gap}(3p) > \text{gap}(3p+1) > 0$ and $\text{gap}(3p+2) = 0$, independently of the morphological characteristics of the lattice. This confers on $A\alpha - T_3$ NRs a behavior closely resembling that of the bulk material⁴, for example, through the emergence of Dirac

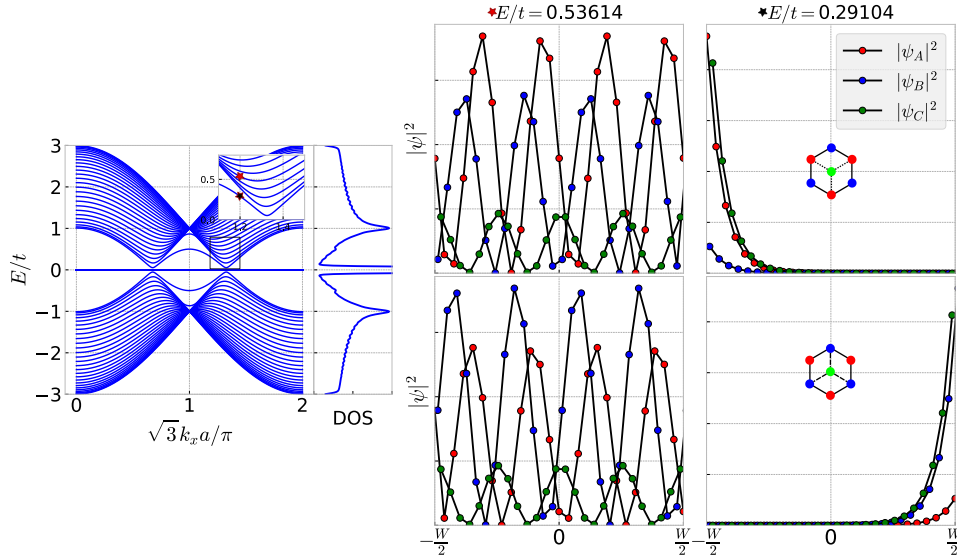
⁴ Bulk material here refers to a system with translational symmetry in all degrees of freedom; in the present case, within the plane.

cones (YAGMURCUKARDES *et al.*, 2016), and in the sense that its band structure is effectively independent of the specific lattice morphology.

3.6 Edge states

Graphene nanoribbons with zigzag terminations exhibit so-called edge states, characterized by an electronic charge density that is predominantly localized at the ribbon edges (WAKABAYASHI *et al.*, 2010). In the figure below, we present the probability density associated with two states belonging to the $3p$ family of $Z\alpha - T_3$ NRs, both with the same wave vector k_x and hopping parameters t_A and t_B . For the state indicated by the red star in the spectrum, the electronic density displays a nodal structure with four pronounced maxima, whereas for the state indicated by the black star, the charge distribution is strongly localized at the nanoribbon edges.

Figure 27 – Probability density of the wave function ψ_j ($j = A, B, C$) corresponding to each sublattice, for the states marked by the red and black stars at wave vector $k = \frac{1.2\pi}{a\sqrt{3}}$, considering the hopping parameters t_A and t_B .



Source: The author.

It is also evident that the type of hopping between neighboring sites significantly influences the probability density. For instance, for the hopping parameter t_A (coupling between sites A and C, see Fig. 15a), the electronic density is enhanced at atomic sites of type A. Conversely, for the hopping t_B (between sites B and C, see Fig. 15b), the electronic density becomes larger at atomic sites of type B. In contrast, the electronic density at

atomic sites of type C remains essentially unchanged and smaller than at the other sites. This behavior arises from the fact that we are considering a transition model with lattice morphology defined by $\theta = \pi/6$.

4 STRAIN IN NANORIBBONS OF $\alpha - T_3$

There exist several approaches to modifying the physical properties of materials; one of the most direct is the mechanical deformation of their underlying crystal structure. The outcome of such deformation depends primarily on the manner in which it is applied and on the intrinsic structural characteristics of the material. For instance, graphene can sustain reversible tensile strains of up to approximately $\sim 20\%$, whereas silicon typically breaks at a strain level of about $\sim 1.5\%$ (SI *et al.*, 2016).

In addition, Dirac materials such as graphene and Weyl semimetals exhibit a distinctive response to non-uniform lattice deformations, namely the emergence of effective (pseudo)magnetic fields induced by these strain fields (LIU; LU, 2022). Taking into account that electronic properties can be tuned via deformation fields, and that the $\alpha - T_3$ lattice interpolates continuously between a Dirac material and a Weyl semimetal. In this chapter, we investigate the effects of uniform deformation on the electronic properties of the $\alpha - T_3$ lattice in both the bulk (infinite system) and nanoribbon (confined system) geometries. Our objective is to perform a systematic analysis of these deformations and their impact on the corresponding electronic structure.

4.1 Strain theory of solids

Within the framework of the theory of infinitesimal (small) deformations, the position vector $\mathbf{R}'$ of a point in a deformed configuration of a (nominally) rigid body is expressed as

$$\mathbf{R}' = (I + \bar{\epsilon} + \bar{\omega}) \mathbf{R}, \quad (4.1)$$

where $\bar{\epsilon}_{ij}$ and $\bar{\omega}_{ij}$ denote, respectively, the strain tensor and the rotation tensor, defined by

$$\bar{\epsilon}_{ij} = \frac{\partial_j u_i + \partial_i u_j}{2}, \quad \bar{\omega}_{ij} = \frac{\partial_j u_i - \partial_i u_j}{2}, \quad (4.2)$$

and $\mathbf{u}$ is the displacement vector field (LURIE, 2010; SADD, 2009; ATKIN; FOX, 2013). The small-strain tensor is a symmetric second-order tensor ($\bar{\epsilon}_{ij} = \bar{\epsilon}_{ji}$) and is commonly represented in matrix form as

$$\bar{\epsilon} = \begin{pmatrix} \epsilon_{xx} & \epsilon_{xy} & \epsilon_{xz} \\ \epsilon_{yx} & \epsilon_{yy} & \epsilon_{yz} \\ \epsilon_{zx} & \epsilon_{zy} & \epsilon_{zz} \end{pmatrix}. \quad (4.3)$$

This tensor comprises three normal and three shear components, giving a total of six independent components that fully characterize small deformations in a linearly elastic solid (SADD, 2009). These components may be grouped into deformations that preserve the body's volume and those that do not. Mathematically, this distinction can be expressed through the following conditions:

$$\det[I + \bar{\epsilon}] = 1 \quad (\text{simple shear and pure shear}), \quad (4.4)$$

$$\det[I + \bar{\epsilon}] \neq 1 \quad (\text{uniaxial and biaxial extension or compression}). \quad (4.5)$$

Representative forms of the strain tensor for these two classes of deformation are given below. For purely shear-type deformations, a typical form is

$$\bar{\epsilon} = \begin{pmatrix} 0 & \epsilon_{xy} & \epsilon_{xz} \\ \epsilon_{yx} & 0 & \epsilon_{yz} \\ \epsilon_{zx} & \epsilon_{zy} & 0 \end{pmatrix}, \quad (4.6)$$

for which only off-diagonal components $\epsilon_{i \neq j}$ are nonzero; these correspond exclusively to shear deformations. In contrast, for purely extensional (normal) deformations, the strain tensor is diagonal,

$$\bar{\epsilon} = \begin{pmatrix} \epsilon_{xx} & 0 & 0 \\ 0 & \epsilon_{yy} & 0 \\ 0 & 0 & \epsilon_{zz} \end{pmatrix}, \quad (4.7)$$

containing only $\epsilon_{i=j}$ terms. In this case, a rectangular material element initially aligned with the principal axes of deformation retains its orthogonal geometry and undergoes only normal (extensional or compressional) strains (SADD, 2009).

In this dissertation, we restrict our attention to planar deformations in the xy -plane. Under this assumption, the strain tensor takes the reduced form

$$\bar{\epsilon} = \begin{pmatrix} \epsilon_{xx} & \epsilon_{xy} & 0 \\ \epsilon_{yx} & \epsilon_{yy} & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad (4.8)$$

which may be regarded as an effectively 2D tensor.

Neglecting rigid-body rotations, the independent in-plane strain components can be classified as follows. The normal (main diagonal) components, ϵ_{xx} and ϵ_{yy} , correspond to uniaxial normal strains in the x - and y -directions, respectively; when they

act simultaneously, they describe a biaxial normal deformation state. The off-diagonal components, ϵ_{xy} and ϵ_{yx} , are associated with shear deformation: taken individually, each contributes to a simple shear strain, while their combined (symmetric) contribution characterizes a state of pure shear strain.

4.2 Strain in real generic lattices

Mechanical strain applied to a lattice induces simultaneous modifications in both the lengths of the nearest-neighbor vectors and the corresponding hopping amplitudes within the TB model. The strained 2D real-space lattice vectors are transformed according to Eq. (4.1). In parallel, the hopping parameters are renormalized by the strain field: t'_{ij} denotes the hopping amplitude between the i -th and j -th atomic sites, located at positions $\mathbf{r}'_i$ and $\mathbf{r}'_j$ in the strained lattice, respectively, and is given by (PEREIRA *et al.*, 2009b)

$$t'_{ij} = t_{ij} \exp \left\{ -\beta \left[\left(\frac{|\mathbf{r}'_i - \mathbf{r}'_j|}{|\mathbf{r}_i - \mathbf{r}_j|} \right) - 1 \right] \right\}, \quad (4.9)$$

where t_{ij} is the hopping amplitude between the sites i and j , located at $\mathbf{r}_i$ and $\mathbf{r}_j$ in the unstrained lattice. In Eq. (2.2), for the α - T_3 lattice, one may adopt the graphene parameters: $\beta = \partial \log t / \partial \log a$ (≈ 3.37) (FILUSCH *et al.*, 2021) is the Grüneisen parameter, while $t = 2.7$ eV and $a = 1.42$ Å correspond to the hopping amplitude and the equilibrium distance, respectively, between nearest-neighbor (NN) sites in unstrained graphene (PEREIRA *et al.*, 2009b).

4.3 Strain in the reciprocal lattice

The reciprocal lattice vectors are constructed from the real-space lattice vectors according to the relation given in Eq. (2.3). To obtain the corresponding strained primitive vectors in reciprocal space, denoted by $\mathbf{b}'_j$, we impose the standard orthogonality condition $\mathbf{r}'_i \cdot \mathbf{b}'_j = 2\pi\delta_{ij}$, which enables us to determine how the strain tensor modifies (or “stretches”) the reciprocal lattice.

We consider strained real-space primitive vectors $\mathbf{r}'_1$, $\mathbf{r}'_2$, and $\mathbf{r}'_3$ that define a generic 2D lattice under tension, embedded in three-dimensional space. The associated strained reciprocal lattice is then characterized by the set of vectors $\{\mathbf{b}'_1, \mathbf{b}'_2, \mathbf{b}'_3\}$ obtained

from the above constraint:

$$\mathbf{b}'_1 = 2\pi \frac{\mathbf{r}'_2 \times \mathbf{r}'_3}{\mathbf{r}'_1 \cdot (\mathbf{r}'_2 \times \mathbf{r}'_3)}, \quad (4.10)$$

$$\mathbf{b}'_2 = 2\pi \frac{\mathbf{r}'_3 \times \mathbf{r}'_1}{\mathbf{r}'_1 \cdot (\mathbf{r}'_2 \times \mathbf{r}'_3)}, \quad (4.11)$$

where

$$\mathbf{r}'_j = \begin{pmatrix} 1 + \epsilon_{xx} & \epsilon_{xy} & 0 \\ \epsilon_{yx} & 1 + \epsilon_{yy} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} r_{jx} \\ r_{jy} \\ r_{jz} \end{pmatrix}. \quad (4.12)$$

To determine $\mathbf{b}'_1$, we first evaluate the cross product $\mathbf{r}'_2 \times \mathbf{r}'_3$:

$$\mathbf{r}'_2 \times \mathbf{r}'_3 = \mathbf{r}'_2 \times \mathbf{r}_3, \quad (4.13)$$

since $\mathbf{r}'_3 = (I + \bar{\epsilon})\mathbf{r}_3 = \mathbf{r}_3 = \hat{z}$. Thus,

$$\begin{aligned} \mathbf{r}'_2 \times \mathbf{r}_3 &= [(I + \bar{\epsilon})\mathbf{r}_2] \times \mathbf{r}_3 \\ &= \begin{pmatrix} \epsilon_{yx}r_{2x} + r_{2y}(\epsilon_{yy} + 1) \\ -\epsilon_{xy}r_{2y} - r_{2x}(\epsilon_{xx} + 1) \\ 0 \end{pmatrix} = \begin{pmatrix} \epsilon_{yy} + 1 & -\epsilon_{yx} & 0 \\ -\epsilon_{xy} & \epsilon_{xx} + 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} (\mathbf{r}_2 \times \mathbf{r}_3). \end{aligned} \quad (4.14)$$

Next, we compute the triple product

$$\begin{aligned} \mathbf{r}'_1 \cdot (\mathbf{r}'_2 \times \mathbf{r}'_3) &= (\epsilon_{xy}r_{1y} + r_{1x}(\epsilon_{xx} + 1))(\epsilon_{yx}r_{2x} + r_{2y}(\epsilon_{yy} + 1)) \\ &\quad + (-\epsilon_{xy}r_{2y} - r_{2x}(\epsilon_{xx} + 1))(\epsilon_{yx}r_{1x} + r_{1y}(\epsilon_{yy} + 1)) \\ &= (r_{1x}r_{2y} - r_{1y}r_{2x})[(\epsilon_{xx} + 1)(\epsilon_{yy} + 1) - \epsilon_{xy}\epsilon_{yx}] \\ &= \det(I + \bar{\epsilon}) \mathbf{r}_1 \cdot (\mathbf{r}_2 \times \mathbf{r}_3). \end{aligned} \quad (4.15)$$

Therefore,

$$\mathbf{b}'_1 = \frac{1}{\det(I + \bar{\epsilon})} \begin{pmatrix} \epsilon_{yy} + 1 & -\epsilon_{yx} & 0 \\ -\epsilon_{xy} & \epsilon_{xx} + 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \mathbf{b}_1. \quad (4.16)$$

For $\mathbf{b}'_2$, we analogously obtain

$$\mathbf{r}'_3 \times \mathbf{r}'_1 = -\mathbf{r}'_1 \times \mathbf{r}_3 = \begin{pmatrix} \epsilon_{yy} + 1 & -\epsilon_{yx} & 0 \\ -\epsilon_{xy} & \epsilon_{xx} + 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} (\mathbf{r}_3 \times \mathbf{r}_1). \quad (4.17)$$

Hence, $\mathbf{b}'_2$ transforms according to the same linear relation as $\mathbf{b}'_1$.

Finally, for truly 2D materials, only two primitive vectors are required to describe the lattice; the third is introduced merely for formal completeness. Consequently, the strain tensor effectively reduces to a 2×2 matrix acting in the plane, and the transformation law for the strained reciprocal lattice vectors simplifies accordingly to the in-plane components of the above relations:

$$\mathbf{b}'_j = [(I + \bar{\epsilon})^{-1}]^T \mathbf{b}_j. \quad (4.18)$$

We observe that it differs from how the real lattice is tensioned.

4.4 Strain in the 2D real lattice

The atomic positions of a strained 2D lattice are represented by transformed basis vectors $\mathbf{r}' = (r'_x, r'_y)$ such that they satisfy (LIMA *et al.*, 2023)

$$\begin{pmatrix} r'_x \\ r'_y \end{pmatrix} = \begin{pmatrix} 1 + \epsilon_{xx} - \sigma\epsilon_{yy} & \epsilon_{xy} \\ \epsilon_{yx} & 1 + \epsilon_{yy} - \sigma\epsilon_{xx} \end{pmatrix} \begin{pmatrix} r_x \\ r_y \end{pmatrix}, \quad (4.19)$$

where $\mathbf{r} = (r_x, r_y)$ denotes the basis vector in the unstrained configuration. The multiplicative factors appearing on the main diagonal account for the contractions or expansions along directions perpendicular to the externally applied load¹

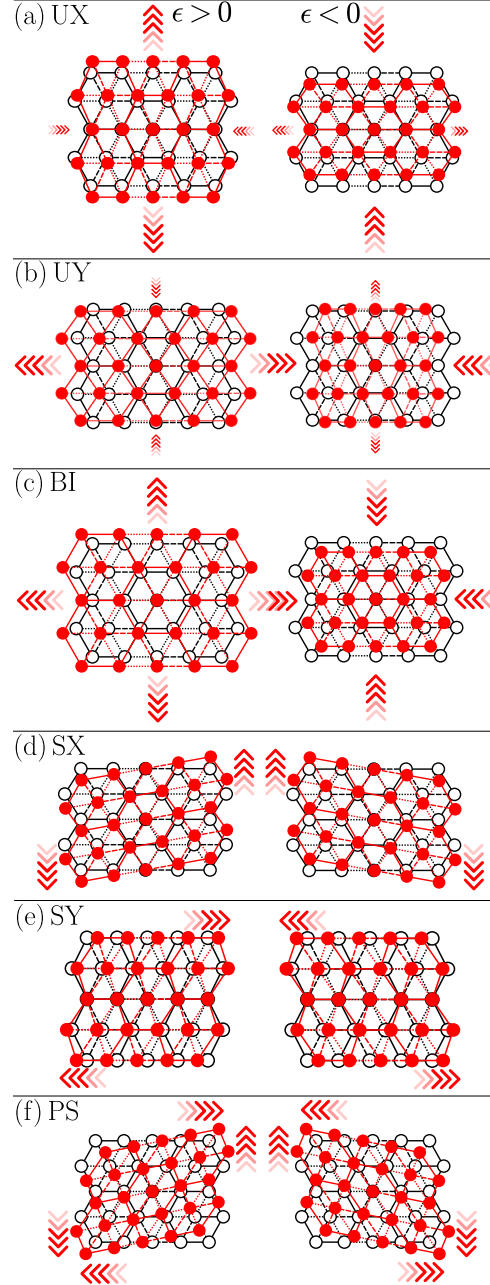
In a 2D lattice, there are six distinct strain configurations that can be imposed: uniaxial tension along the x direction (UX), uniaxial tension along the y direction (UY), biaxial tension (BI), simple shear with principal axis along x (SX), simple shear with principal axis along y (SY), and pure shear (PS) (LIMA *et al.*, 2023). The corresponding non-vanishing components of the strain tensor are summarized in Table 8.

Table 8 – Non-zero components of the strain tensor [Eq. (4.14)] for each type of deformation applied to the $\alpha - T_3$ lattice.

Type of strain	ϵ_{xx}	ϵ_{xy}	ϵ_{yx}	ϵ_{yy}
UX	ϵ	0	0	0
UY	0	0	0	ϵ
BI	ϵ	0	0	ϵ
SX	0	ϵ	0	0
SY	0	0	ϵ	0
PS	0	ϵ	ϵ	0

¹ The parameter σ is the Poisson transverse contraction coefficient, which characterizes the material response to deformations in directions orthogonal to the applied strain (PEREIRA *et al.*, 2009a). For a more detailed visualization, see Fig. 28.

Figure 28 – Comparison between the undeformed $\alpha - T_3$ lattice (black circles) and the strained lattice (red circles), for tensile strain $\epsilon > 0$ (left) and compressive strain $\epsilon < 0$ (right). Panels correspond to: (a) UX strain, (b) UY strain, (c) BI strain, (d) SX strain, (e) SY strain, and (f) PS strain. The finite Poisson ratio accounts for the transverse compression or extension in the vertical (horizontal) direction under UX (UY) loading.



Source: The author.

A schematic representation of the effect of these six types of strain on the $\alpha - T_3$ lattice is shown in Fig. 28.

We now determine the mathematically admissible values of ϵ for each strain configuration, ensuring the absence of singularities when analyzing the existence of critical

values for band-gap opening in the material's electronic band structure. From Eq. (4.13), the required condition is

$$\det(I + \bar{\epsilon}) \neq 0, \quad (4.20)$$

so that

$$\begin{aligned} \det(I + \bar{\epsilon}) &= \begin{vmatrix} 1 + \epsilon_{xx} - \sigma\epsilon_{yy} & \epsilon_{xy} \\ \epsilon_{yx} & 1 + \epsilon_{yy} - \sigma\epsilon_{xx} \end{vmatrix} \\ &= (1 + \epsilon_{xx} - \sigma\epsilon_{yy})(1 + \epsilon_{yy} - \sigma\epsilon_{xx}) - \epsilon_{yx}\epsilon_{xy} \neq 0. \end{aligned} \quad (4.21)$$

Using the strain parametrizations listed in Table 8, we obtain the corresponding constraints on ϵ for the six strain types, which are summarized in the table below.

Table 9 – Restrictions on the values of ϵ for the six types of strain.

Type of strain	Restriction
UX	$\epsilon \neq -1, \sigma^{-1}$
UY	$\epsilon \neq -1, \sigma^{-1}$
BI	$\epsilon \neq (\sigma - 1)^{-1}$
SX	No restrictions
SY	No restrictions
PS	$\epsilon \neq \pm 1$

Although these constraints were derived from a purely mathematical requirement, namely the non-vanishing of the determinant of the deformation tensor, they also possess a clear physical interpretation. In the uniaxial cases, for instance, stretching (compressing) up to $\epsilon = \sigma^{-1}$ ($\epsilon = -1$) corresponds to a deformation in which neighboring atomic sites are driven into mutual overlap. An analogous situation occurs for the BI and PS configurations at their respective excluded values of ϵ . The only exceptions are the simple shear deformations, for which the applied strain does not induce overlap between atomic sites and therefore does not lead to such singular configurations.

4.4.1 The tight-binding Hamiltonian for the strained $\alpha - T_3$ Lattice

The TB Hamiltonian for the strained $\alpha - T_3$ lattice is

$$\sum_{i \neq j} t'_{ij} g_i^\dagger g_j + h.c. = \sum_{i,j} t'_{ij} (\hat{a}_i^\dagger \hat{b}_j + \hat{b}_j^\dagger \hat{a}_i) + \sum_{j,l} t'_{jl} (\hat{a}_j^\dagger \hat{c}_l + \hat{c}_l^\dagger \hat{a}_j) + \sum_{l,m} t'_{lm} (\hat{b}_l^\dagger \hat{c}_m + \hat{c}_m^\dagger \hat{b}_l), \quad (4.22)$$

where $\hat{g}_i$ ($\hat{g}_i^\dagger$) with $g = a, b, c$ are annihilation (creation) operators at site i , and t'_{ij} is the strained hopping parameter,

$$t'_{ij} = t_{ij} e^{-\beta(|\mathbf{r}'_i - \mathbf{r}'_j|/|\mathbf{r}_i - \mathbf{r}_j| - 1)} \quad \mathbf{r}' = (I + \bar{\epsilon})\mathbf{r}. \quad (4.23)$$

Expressing the operators in momentum space for $A \rightarrow B$ hoppings,

$$\sum_{i,j} t'_{ij} \hat{a}_i^\dagger \hat{b}_j = \sum_{i,j} t'_{ij} \left(\frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\mathbf{k} \cdot \mathbf{r}'_i} \hat{a}_{\mathbf{k}}^\dagger \right) \left(\frac{1}{\sqrt{N}} \sum_{\mathbf{k}''} e^{i\mathbf{k}'' \cdot \mathbf{r}'_j} \hat{b}_{\mathbf{k}''} \right), \quad (4.24)$$

and permuting the sums gives

$$\sum_{i,j} t'_{ij} \hat{a}_i^\dagger \hat{b}_j = \sum_{\mathbf{k}, \mathbf{k}''} \frac{1}{N} \sum_{i,j} t_{ij} e^{-\beta(|\mathbf{r}'_i - \mathbf{r}'_j|/|\mathbf{r}_i - \mathbf{r}_j| - 1)} e^{-i\mathbf{k} \cdot \mathbf{r}'_i} e^{i\mathbf{k}'' \cdot \mathbf{r}'_j} \hat{a}_{\mathbf{k}}^\dagger \hat{b}_{\mathbf{k}''}, \quad (4.25)$$

which can be rewritten as

$$\sum_{i,j} \hat{a}_i^\dagger \hat{b}_j = t \sum_{\mathbf{k}, \mathbf{k}''} \frac{1}{N} \sum_{i,j} t_{ij} e^{-\beta(|\mathbf{d}'_{ij}|/|\mathbf{d}_{ij}| - 1)} e^{i(\mathbf{k}'' - \mathbf{k}) \cdot \mathbf{r}'_i} e^{-i\mathbf{k}'' \cdot \mathbf{d}'_{ij}} \hat{a}_{\mathbf{k}}^\dagger \hat{b}_{\mathbf{k}''}, \quad (4.26)$$

where $\mathbf{d}'_{ij} = \mathbf{r}'_i - \mathbf{r}'_j$ is the position of sublattice A relative to sublattice B . We now keep i fixed and sum over j , thus

$$\begin{aligned} \sum_{i,j} t'_{ij} (\hat{a}_i^\dagger \hat{b}_j) &= \sum_{\mathbf{k}, \mathbf{k}''} \underbrace{\sum_i \frac{1}{N} e^{i(\mathbf{k}'' - \mathbf{k}) \cdot \mathbf{r}'_i}}_{=\delta_{\mathbf{k}, \mathbf{k}''}} \sum_{n=1}^3 t e^{-\beta \left(\frac{|\mathbf{d}'_n|}{|\mathbf{d}_n|} - 1 \right)} e^{-i\mathbf{k}'' \cdot \mathbf{d}_n} \hat{a}_{\mathbf{k}}^\dagger \hat{b}_{\mathbf{k}''} \\ &= t \sum_{\mathbf{k}} f_{AB}(\mathbf{k}) \hat{a}_{\mathbf{k}}^\dagger \hat{b}_{\mathbf{k}}, \end{aligned} \quad (4.27)$$

where, within the nearest-neighbor approximation²,

$$f_{AB}(\mathbf{k}) = \sum_{n=1}^3 e^{-\beta \left(\frac{|(I+\bar{\epsilon})\mathbf{d}_n|}{|\mathbf{d}_n|} - 1 \right)} e^{-i\mathbf{k} \cdot [(I+\bar{\epsilon})\mathbf{d}_n]}, \quad (4.28)$$

and, using the hermiticity condition $\left(\sum_{i,j} t'_{ij} \hat{a}_i^\dagger \hat{b}_j \right)^\dagger = \sum_{i,j} t'_{ji} \hat{b}_j^\dagger \hat{a}_i$, one obtains

$$f_{BA}(\mathbf{k}) = f_{AB}(\mathbf{k})^* = \sum_{n=1}^3 e^{-\beta \left(\frac{|(I+\bar{\epsilon})\mathbf{d}_n|}{|\mathbf{d}_n|} - 1 \right)} e^{i\mathbf{k} \cdot [(I+\bar{\epsilon})\mathbf{d}_n]}. \quad (4.29)$$

By proceeding analogously for the remaining sublattice pairs, we obtain

$$f_{AC}(\mathbf{k}) = f_{CA}(\mathbf{k})^* = \sum_{n=1}^3 e^{-\beta \left(\frac{|(I+\bar{\epsilon})\mathbf{d}_n|}{|\mathbf{d}_n|} - 1 \right)} e^{i\mathbf{k} \cdot [(I+\bar{\epsilon})\mathbf{d}_n]}, \quad (4.30)$$

² $\mathbf{d}_1 = (0 \quad 1)^T a$, $\mathbf{d}_2 = (-\sqrt{3} \quad -1)^T a/2$ and $\mathbf{d}_3 = (\sqrt{3} \quad -1)^T a/2$

$$f_{BC}(\mathbf{k}) = f_{CB}(\mathbf{k})^* = \sum_{n=1}^3 e^{-\beta \left(\frac{|(I+\bar{\epsilon})\mathbf{d}_n|}{|\mathbf{d}_n|} - 1 \right)} e^{-i\mathbf{k} \cdot [(I+\bar{\epsilon})\mathbf{d}_n]}. \quad (4.31)$$

Thus, the TB Hamiltonian of the strained $\alpha - T_3$ lattice can be written as

$$H = \begin{pmatrix} E_A & t f_{AB}(\mathbf{k}) & \alpha t_A f_{AC}^*(\mathbf{k}) \\ t f_{AB}^*(\mathbf{k}) & E_B & \alpha t_B f_{BC}(\mathbf{k}) \\ \alpha t_A f_{AC}(\mathbf{k}) & \alpha t_B f_{BC}^*(\mathbf{k}) & E_C \end{pmatrix}. \quad (4.32)$$

To determine the energy spectrum of the strained lattice, we diagonalize the Hamiltonian by solving

$$\begin{aligned} \det(H - \lambda I) &= \begin{vmatrix} E_A - \lambda & t f_{AB}(\mathbf{k}) & \alpha t_A f_{AC}^*(\mathbf{k}) \\ t f_{AB}^*(\mathbf{k}) & E_B - \lambda & \alpha t_B f_{BC}(\mathbf{k}) \\ \alpha t_A f_{AC}(\mathbf{k}) & \alpha t_B f_{BC}^*(\mathbf{k}) & E_C - \lambda \end{vmatrix} \\ &= (E_A - \lambda)(E_B - \lambda)(E_C - \lambda) \\ &\quad + \alpha^2 t t_A t_B (f_{AB} f_{AC} f_{BC} + f_{AB}^* f_{AC}^* f_{BC}^*) \\ &\quad - (E_A - \lambda) \alpha^2 t_B^2 |f_{BC}|^2 - (E_B - \lambda) \alpha^2 t_A^2 |f_{AC}|^2 - (E_C - \lambda) t^2 |f_{AB}|^2. \end{aligned} \quad (4.33)$$

Let us now consider a simplified situation characterized by $E_A = E_B = E_C = E$ and $t_A = t$, together with either $t_B = 0$ or $t_A = 0$ and $t_B = t$. In this case, the eigenvalues reduce to

$$\lambda_0(\mathbf{k}) = E, \quad \lambda_{\pm}(\mathbf{k}) = E \mp t |f(\mathbf{k})| \sqrt{\alpha^2 + 1}, \quad (4.34)$$

where

$$f(\mathbf{k}) = \sum_{n=1}^3 e^{-\beta \left(\frac{|(I+\bar{\epsilon})\mathbf{d}_n|}{|\mathbf{d}_n|} - 1 \right)} e^{-i\mathbf{k} \cdot [(I+\bar{\epsilon})\mathbf{d}_n]}. \quad (4.35)$$

Consequently, we conclude that the specific form of the coupling between the central site (C) and its nearest neighbors, characterized by the hopping parameters t_A and t_B [see Fig. 16], does not alter the band structure in the case of an infinite lattice, provided that the sublattices share identical on-site energies. Furthermore, we observe that the flat band in the nearest-neighbor model of the $\alpha - T_3$ lattice is not affected by any deformation [Eq. (4.34)], and the electron-hole symmetry [$\lambda_+(\mathbf{k}) = -\lambda_-(\mathbf{k})$] is likewise preserved in the strained lattice [Eq. (4.34)].

In conclusion, for an infinite $\alpha - T_3$ lattice with equal on-site energies on all three sublattices, the specific pattern of coupling between the hub (central) site and its

nearest neighbors does not alter the band structure. Furthermore, within the nearest-neighbor approximation, the perfectly flat band of the $\alpha - T_3$ lattice is not affected by any deformation and the electron–hole symmetry of the spectrum is preserved.

4.4.2 *Energy gap of the $\alpha - T_3$ lattice as a function of the parameter ϵ*

The energy spectrum of the $\alpha - T_3$ lattice exhibits a characteristic three-band structure with particle–hole symmetry, analogous to the symmetric valence and conduction bands observed in graphene. Within this framework, and owing to the particle–hole symmetry, we define the energy gap of the $\alpha - T_3$ lattice as the absolute difference between the minimum energy of the conduction band and the energy of the flat band as sketched in the inset of Fig. 29(c). Figures 29(a)-29(f) present the dimensionless energy gap, $\Delta E_{\text{gap}}/t$, as a function of ϵ for the UX, UY, BI, SX, SY, and PS strains, and for selected values of the morphological parameter α .

It is observed that only the BI strain is unable to induce an energy gap in the band structure of the $\alpha - T_3$ lattice; all other strain configurations result in gap opening. In particular, the UX strain produces a gap for positive strain values, with a critical strain of approximately $\epsilon \approx 0.23$, whereas the UY strain induces a gap only for negative strain, with a critical value of approximately $\epsilon \approx -0.23$. Thus, UX and UY share the same critical strain magnitude, although the gap increases more rapidly as a function of $|\epsilon|$ for the UY case. For the remaining strain configurations, the gap-opening behavior is symmetric with respect to the ϵ -axis, i.e., an energy gap is generated whenever $|\epsilon|$ exceeds the corresponding critical value, independent of the sign of ϵ .

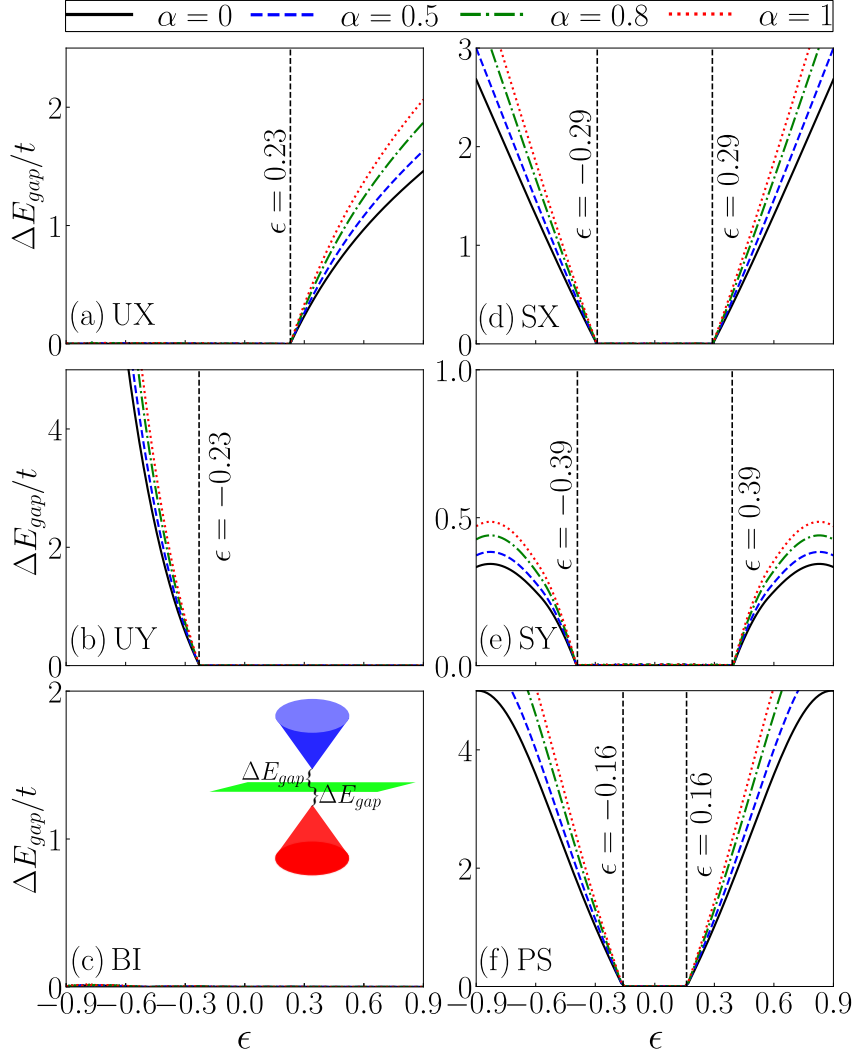
Furthermore, the critical strain values for gap opening are identical for different values of α . This follows from the fact that the gap of the $\alpha - T_3$ lattice can be expressed in terms of the graphene energy gap as

$$Gap_{\alpha-T_3}(\epsilon) = \left| \min_{\mathbf{k}} \lambda_+(\mathbf{k}) - E \right|, \quad (4.36)$$

where λ_+ and E are the eigenvalues defined in Eq. (4.29). In contrast, the graphene gap is given by

$$Gap_{\text{graphene}} = \left| \min_{\mathbf{k}} \lambda_+(\mathbf{k}) - \max_{\mathbf{k}} \lambda_-(\mathbf{k}) \right|. \quad (4.37)$$

Figure 29 – Energy gap ($\Delta E_{\text{gap}}/t$) of the strained α - T_3 dispersion as a function of the strain amplitude ϵ for $\alpha = 0$ (black solid curve), $\alpha = 0.5$ (blue dashed curve), $\alpha = 0.8$ (green dash-dotted curve), and $\alpha = 1$ (red dotted curve), under (a) UX strain applied along the zigzag direction, (b) UY strain applied along the armchair direction, (c) BI strain, (d) SX strain applied along the zigzag direction, (e) SY strain applied along the armchair direction, and (f) PS strain imposed on the α - T_3 lattice. The vertical gray dashed lines indicate the critical strain amplitude ϵ_c at which an energy gap opens in the electronic band structure.



Source: The author.

After straightforward algebraic manipulations, one obtains

$$Gap_{\alpha-T_3}(\epsilon) = \left| \min_{\mathbf{k}} \lambda_+(\mathbf{k}) - E \right| = \frac{\sqrt{\alpha^2 + 1}}{2} Gap_{\text{graphene}}. \quad (4.38)$$

Therefore, the energy gap of the $\alpha - T_3$ lattice is proportional to the graphene energy gap, which explains the behavior observed in Fig. 29. The critical conditions for the onset of an energy gap are identical to those of graphene; however, in the present context, they additionally encode the dependence of the gap on the hopping amplitudes between

neighboring sites. In Ref. (HASEGAWA *et al.*, 2006), titled “Zero modes of TB electrons on the honeycomb lattice”, the authors derived the following inequality for the nearest-neighbor hopping parameters:

$$|t_1 - t_2| \leq |t_3| \leq |t_1 + t_2|, \quad (4.39)$$

such that, when this condition is satisfied, the band structure remains gapless and the isotropy of the lattice is preserved. In an analogous manner, we now verify this relation for the $\alpha - T_3$ lattice. To this end, we consider the eigenvalues in Eq. (4.34), which can be rewritten as

$$\lambda = 0, \quad \lambda^2 = (\alpha^2 + 1) \left| \sum_{n=1}^3 t_n f_n(\mathbf{k}) \right|^2, \quad (4.40)$$

where t_n and $f_n(\mathbf{k})$ denote, respectively, the hopping amplitude between lattice sites and the structure factor associated with a site that is not equivalent under deformation. These quantities are given by

$$t_n = t_0 \exp \left[-\beta \left(\frac{|(I + \bar{\epsilon})\mathbf{d}_n|}{|\mathbf{d}_n|} - 1 \right) \right], \quad (4.41)$$

$$f_n(\mathbf{k}) = \exp \left[-i\mathbf{k} \cdot (I + \bar{\epsilon})\mathbf{d}_n \right]. \quad (4.42)$$

We now analyze the eigenvalues associated with the conduction and valence bands by expanding the terms in Eq. (4.40):

$$\begin{aligned} \lambda^2 &= (\alpha^2 + 1) \left| \sum_{n=1}^3 t_n f_n(\mathbf{k}) \right|^2 \\ &= (\alpha^2 + 1) \left(\sum_{n=1}^3 t_n f_n(\mathbf{k}) \right) \left(\sum_{n=1}^3 t_n f_n(\mathbf{k}) \right)^* \\ &= (\alpha^2 + 1) \left[t_1^2 |f_1|^2 + t_2^2 |f_2|^2 + t_3^2 |f_3|^2 + t_1 t_2 (f_1 f_2^* + f_2 f_1^*) \right. \\ &\quad \left. + t_1 t_3 (f_1 f_3^* + f_3 f_1^*) + t_2 t_3 (f_2 f_3^* + f_3 f_2^*) \right]. \end{aligned} \quad (4.43)$$

Since $|f_n|^2 = 1$, this simplifies to

$$\begin{aligned} \lambda^2 &= (\alpha^2 + 1) \left[t_1^2 + t_2^2 + t_3^2 + t_1 t_2 (f_1 f_2^* + f_2 f_1^*) \right. \\ &\quad \left. + t_1 t_3 (f_1 f_3^* + f_3 f_1^*) + t_2 t_3 (f_2 f_3^* + f_3 f_2^*) \right]. \end{aligned} \quad (4.44)$$

Using the identity $\mathbf{k} \cdot [(I + \bar{\epsilon})\mathbf{d}_n] = [(I + \bar{\epsilon})^T \mathbf{k}] \cdot \mathbf{d}_n = \mathbf{k}' \cdot \mathbf{d}_n$, we can write

$$f_n = \exp \left[-i\mathbf{k}' \cdot \mathbf{d}_n \right]. \quad (4.45)$$

For the $\alpha - T_3$ lattice in our model, the nearest-neighbor vectors are given by $\mathbf{d}_1 = (0 \ 1)^T a$, $\mathbf{d}_2 = (-\sqrt{3} \ -1)^T a/2$, and $\mathbf{d}_3 = (\sqrt{3} \ -1)^T a/2$, which leads to

$$f_1 = \exp(-iak'_{0y}), \quad (4.46)$$

$$f_2 = \exp\left[\frac{ia}{2}(\sqrt{3}k'_{0x} + k'_{0y})\right], \quad (4.47)$$

$$f_3 = \exp\left[-\frac{ia}{2}(\sqrt{3}k'_{0x} - k'_{0y})\right]. \quad (4.48)$$

Consequently, the terms in parentheses in Eq. (4.44) are

$$f_1 f_2^* + f_2 f_1^* = e^{ia\left(\frac{\sqrt{3}}{2}k'_{0x} + \frac{3}{2}k'_{0y}\right)} + e^{-ia\left(\frac{\sqrt{3}}{2}k'_{0x} + \frac{3}{2}k'_{0y}\right)} = 2 \cos\left(\frac{a\sqrt{3}}{2}k'_{0x} + \frac{3a}{2}k'_{0y}\right),$$

$$f_1 f_3^* + f_3 f_1^* = e^{ia\left(-\frac{\sqrt{3}}{2}k'_{0x} + \frac{3}{2}k'_{0y}\right)} + e^{-ia\left(-\frac{\sqrt{3}}{2}k'_{0x} + \frac{3}{2}k'_{0y}\right)} = 2 \cos\left(-\frac{a\sqrt{3}}{2}k'_{0x} + \frac{3a}{2}k'_{0y}\right),$$

$$f_2 f_3^* + f_3 f_2^* = e^{ia(-\sqrt{3}k'_{0x})} + e^{-ia(\sqrt{3}k'_{0x})} = 2 \cos(-\sqrt{3}ak'_{0x}).$$

By defining

$$2\pi k'_1 = \frac{a\sqrt{3}}{2}k'_{0x} + \frac{3a}{2}k'_{0y}, \quad 2\pi k'_2 = -\frac{a\sqrt{3}}{2}k'_{0x} + \frac{3a}{2}k'_{0y},$$

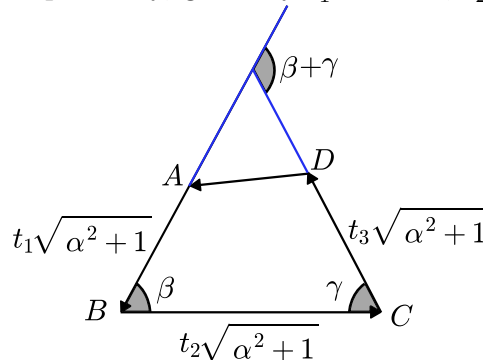
we obtain

$$\begin{aligned} \lambda^2 = (\alpha^2 + 1) & \left[t_1^2 + t_2^2 + t_3^2 + 2t_1 t_2 \cos(2\pi k'_1) + 2t_1 t_3 \cos(2\pi k'_2) \right. \\ & \left. + 2t_2 t_3 \cos[2\pi(k'_1 - k'_2)] \right]. \end{aligned} \quad (4.49)$$

Having obtained this expression, we now proceed to determine its minimum value $|\lambda_{\mathbf{k}}|$.

For this purpose, we consider the following quadrilateral,

Figure 30 – Schematic illustration used to explain the emergence of zero modes in the band dispersion of the $\alpha - T_3$ lattice. The moduli of the vectors $\mathbf{AB}$, $\mathbf{BC}$, and $\mathbf{CD}$ are, respectively, given by $t'_1\sqrt{\alpha^2 + 1}$, $t'_2\sqrt{\alpha^2 + 1}$, and $t'_3\sqrt{\alpha^2 + 1}$.



Source: Figure adapted from
Ref. (HASEGAWA *et al.*, 2006).

In this construction, the moduli of the sides are determined by the hopping parameters in the presence of deformation. The squared modulus of the vector $\mathbf{DA}$ can be written as

$$\begin{aligned} |\mathbf{DA}|^2 &= |\mathbf{AB} + \mathbf{BC} + \mathbf{CD}|^2 \\ &= \mathbf{AB} \cdot (\mathbf{AB} + \mathbf{BC} + \mathbf{CD}) + \mathbf{BC} \cdot (\mathbf{AB} + \mathbf{BC} + \mathbf{CD}) \\ &\quad + \mathbf{CD} \cdot (\mathbf{AB} + \mathbf{BC} + \mathbf{CD}). \end{aligned} \quad (4.50)$$

Carrying out the scalar products explicitly,³ we obtain

$$|\mathbf{DA}|^2 = t_1^2 + t_2^2 + t_3^2 + 2t_1t_2 \cos(\pi - \beta) + 2t_1t_3 \cos(\beta + \gamma) + 2t_2t_3 \cos(\pi - \gamma). \quad (4.51)$$

After some straightforward algebraic manipulations, this expression can be recast as

$$\begin{aligned} |\mathbf{DA}|^2 &= (\alpha^2 + 1) [t_1^2 + t_2^2 + t_3^2 - 2t_1t_2 \cos \beta - 2t_1t_3 \cos(\pi - \beta - \gamma) \\ &\quad - 2t_2t_3 \cos \gamma], \end{aligned} \quad (4.52)$$

and by choosing

$$\beta = \pi - 2\pi k_1' \quad \text{and} \quad \gamma = \pi + 2\pi(k_1' - k_2'), \quad (4.53)$$

we recover the same mathematical relation obtained in Eq. (4.49). Geometrically, this condition implies the inequality

$$\begin{aligned} (\alpha^2 + 1) \Big[t_1^2 + t_2^2 + t_3^2 + 2t_1t_2 \cos(2\pi k_1') + 2t_1t_3 \cos(2\pi k_2') \\ + 2t_2t_3 \cos(2\pi(k_1' - k_2')) \Big] \geq 0. \end{aligned} \quad (4.54)$$

Equality is attained when

$$\cos(2\pi k_1') = \frac{t_3^2 - t_1^2 - t_2^2}{2t_1t_2}, \quad (4.55)$$

$$\cos(2\pi k_2') = \frac{t_2^2 - t_1^2 - t_3^2}{2t_1t_3}, \quad (4.56)$$

$$\cos[2\pi(k_1' - k_2')] = \frac{t_1^2 - t_2^2 - t_3^2}{2t_2t_3}, \quad (4.57)$$

which corresponds to the situation in which the quadrilateral depicted in Fig. 30 degenerates into a triangle. This triangular configuration is characterized by the standard triangle inequality

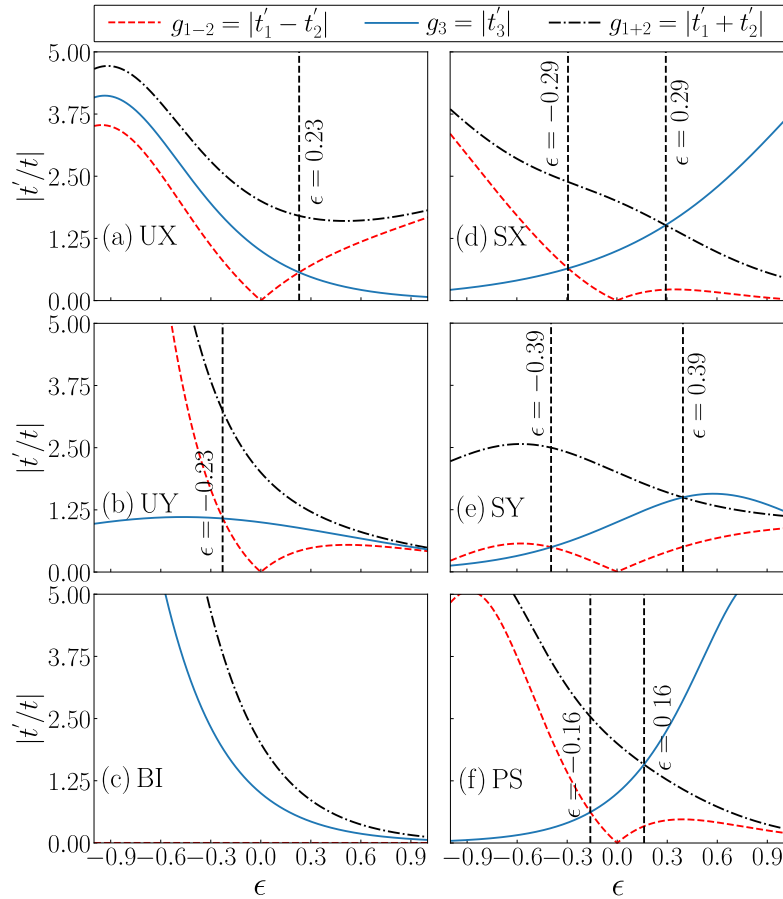
$$|t_1 - t_2| \leq |t_3| \leq |t_1 + t_2|. \quad (4.58)$$

³ Here, β denotes the geometric angle indicated in Fig. 30, and should not be confused with the Grüneisen parameter.

In conclusion, this geometric analysis shows that the critical conditions for band-gap opening in the $\alpha - T_3$ model coincide with those of graphene and are therefore independent of the morphological parameter α .

To identify the regions in which an energy gap opens, we analyze the behavior of the functions $g_{1\pm 2}(\epsilon) = |t_1 \pm t_2|$ and $g_3(\epsilon) = |t_3|$ as a function of the strain parameter ϵ . These functions are represented in Fig. 31.

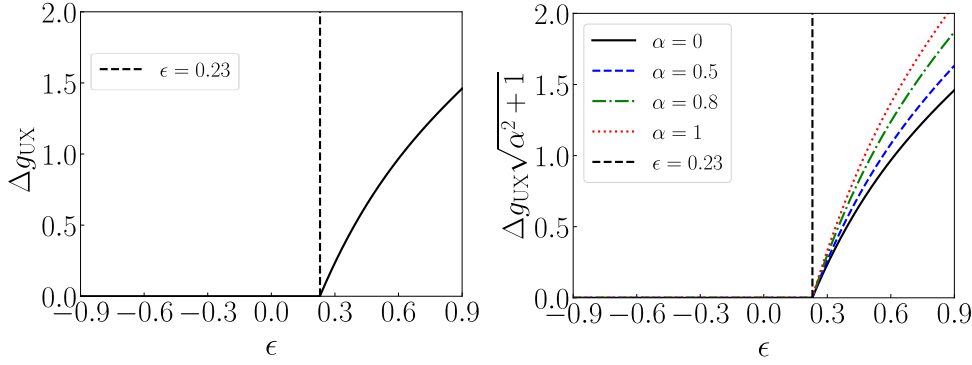
Figure 31 – Terms of the Hasegawa inequality [Eq. (4.58)] $g_{1-2}(\epsilon) = |t'_1 - t'_2|$ (red dashed curves), $g_3(\epsilon) = |t'_3|$ (blue solid curves), and $g_{1+2}(\epsilon) = |t'_1 + t'_2|$ (black dash-dotted curves), as a function of strain amplitude ϵ , when the (a) UX-strain applied in zigzag-direction, (b) UY-strain applied in armchair-direction, (c) BI-strain, (d) SX-strain applied in zigzag-direction, (e) SY-strain applied in armchair-direction, and (f) PS-strain, acts on the $\alpha - T_3$ lattice. The vertical dashed-black lines mark the intersection between the two curves and correspond to the critical points for the gap opening ϵ_c .



Source: The author.

From Fig. 31, we observe that the critical points associated with the opening of the energy gap (indicated by vertical dashed-black lines) occur precisely when the inequality is violated. This behavior is found for uniaxial and shear strains; the only

Figure 32 – Normalized gap-related quantities as a function of ϵ for UX strain.
 (a) Δg_{UX} . (b) $\Delta g_{\text{UX}}\sqrt{\alpha^2 + 1}$.



Source: The author.

exception is the biaxial strain, for which the inequality (4.57) is always satisfied. The functions $g_{1\pm 2}(\epsilon) = |t_1 \pm t_2|$ and $g_3(\epsilon) = |t_3|$, shown in Fig. 31, therefore provide the exact critical values of ϵ at which an energy gap emerges in the lattice band structure. Taking this property into account, we next analyze, for each type of strain, the behavior of the corresponding curves in the vicinity of the critical point.

For uniaxial strain along the x direction (UX strain), we define

$$\Delta g_{\text{UX}} = \frac{|t_1 - t_2| - |t_3|}{t} \geq 0, \quad (4.59)$$

which is plotted in Fig. 32a. It is evident that Fig. 32a exhibits the same qualitative behavior as the lattice gap energy $\alpha - T_3$ in the limiting case $\alpha = 0$, as shown in Fig. 29. Using Eq. (4.38), we can then express the band gap, measured from the critical point, for uniaxial deformation along the x direction as

$$\frac{\Delta E_{\text{gap,UX}}}{t} = \Delta g_{\text{UX}}\sqrt{\alpha^2 + 1} = \sqrt{\alpha^2 + 1} \frac{|t_1 - t_2| - |t_3|}{t}, \quad (4.60)$$

whose graphical representation is shown in Fig. 32b. This result is in agreement with the numerical data previously obtained in Fig. 29. In general, the energy gaps induced by the deformations UX, UY, SX, SY, and PS can be expressed analytically as

$$\Delta E_{\text{gap}} = \sqrt{\alpha^2 + 1} (|t_1 - t_2| - |t_3|) f_{\epsilon, \epsilon_{\pm}}, \quad \text{UX}(+), \text{UY}(-), \quad (4.61a)$$

$$\Delta E_{\text{gap}} = \sqrt{\alpha^2 + 1} [(|t_3| - |t_1 + t_2|) f_{\epsilon, \epsilon_+} + (|t_1 - t_2| - |t_3|) f_{\epsilon, \epsilon_-}], \quad \text{SX, SY, PS}(\pm). \quad (4.61b)$$

where the functions $f_{\epsilon, \epsilon_{\pm}}$ select, respectively, the positive and negative strain-amplitude intervals beyond the critical point ϵ_c . To elucidate the role of $f_{\epsilon, \epsilon_{\pm}}$ more clearly, we reconsider the UX configuration. Prior to the critical strain for gap opening ($\epsilon \approx 0.23$), one

has $\Delta E_{gap} = 0$, even though $\sqrt{\alpha^2 + 1} (|t_1 - t_2| - |t_3|) < 0$ (and is, in particular, nonzero). For Eq. (4.61a) to consistently represent the energy gap, it is therefore necessary that $f_{\epsilon, \epsilon_+} = 0$ for $\epsilon < \epsilon_c$.

For strains exceeding the critical value, $\epsilon > \epsilon_c$, the gap becomes

$$\Delta E_{gap} = \sqrt{\alpha^2 + 1} (|t_1 - t_2| - |t_3|) > 0,$$

which implies $f_{\epsilon, \epsilon_+} = 1$ in this regime. Hence, f_{ϵ, ϵ_+} exhibits a behavior analogous to the Heaviside step function $\Theta(x)$, whose defining properties are

$$\Theta(x) = \begin{cases} 0, & x < 0, \\ 1, & x \geq 0. \end{cases} \quad (4.62)$$

At the critical point $\epsilon = \epsilon_c$, where $|t_1 - t_2| = |t_3|$, one can define $f_{\epsilon, \epsilon_+} \equiv \Theta(|t_1 - t_2| - |t_3|)$. More generally, whenever Eq. (4.58) is not satisfied, the evolution of the energy gap is determined by the competition among the functions $g_{1-2}(\epsilon) = |t_1 - t_2|$, $g_{1+2}(\epsilon) = |t_1 + t_2|$, and $g_3(\epsilon) = |t_3|$ entering the Hasegawa inequality, all multiplied by the global factor $\sqrt{1 + \alpha^2}$. Consequently, the energy gap of the α - T_3 lattice can be expressed in the compact form

$$\begin{aligned} \Delta E_{gap} = \sqrt{\alpha^2 + 1} & \left[(|t_1 - t_2| - |t_3|) \Theta(|t_1 - t_2| - |t_3|) \right. \\ & \left. + (|t_3| - |t_1 + t_2|) \Theta(|t_3| - |t_1 + t_2|) \right], \end{aligned} \quad (4.63)$$

where Θ denotes the Heaviside step function, enforcing the vanishing of the energy gap whenever the Hasegawa inequality [Eq. (4.58)] is satisfied.

The analytic expression given by Eq. (4.63) demonstrates that, once the critical point for gap opening is exceeded, the relative values of the hopping amplitudes are the sole quantities determining the evolution of the energy gap, as the latter becomes independent of the structure factor. This result, although strictly valid only for very large deformations beyond the elastic regime of graphene, is, to the best of our knowledge, unprecedented in the literature, and remains unchanged even if the strain-induced hopping expansion in Eq. (4.9) is modified.

The contour plots of the energy bands, together with the first Brillouin zones of the unstrained (black dotted line) and strained (white dotted line) α - T_3 lattice for the six strain configurations and selected values of ϵ , are presented in the figures below.

The constant-energy contours (black lines) in the conduction and valence bands depict isoenergetic lines in the vicinity of the Fermi level and correspond to the normalized energies $E/t = 0.1, 0.2, 0.4, 0.6$, and 0.8 . The contour plots are shown for the intermediate-coupling regime, characterized by $\alpha = 0.5$, since for other values of α it suffices to rescale the energy spectrum accordingly. As established previously, within the nearest-neighbor tight-binding approximation, the qualitative structure of the band dispersion is equivalent to that of graphene and differs only by an overall multiplicative factor of $\sqrt{\alpha^2 + 1}$.

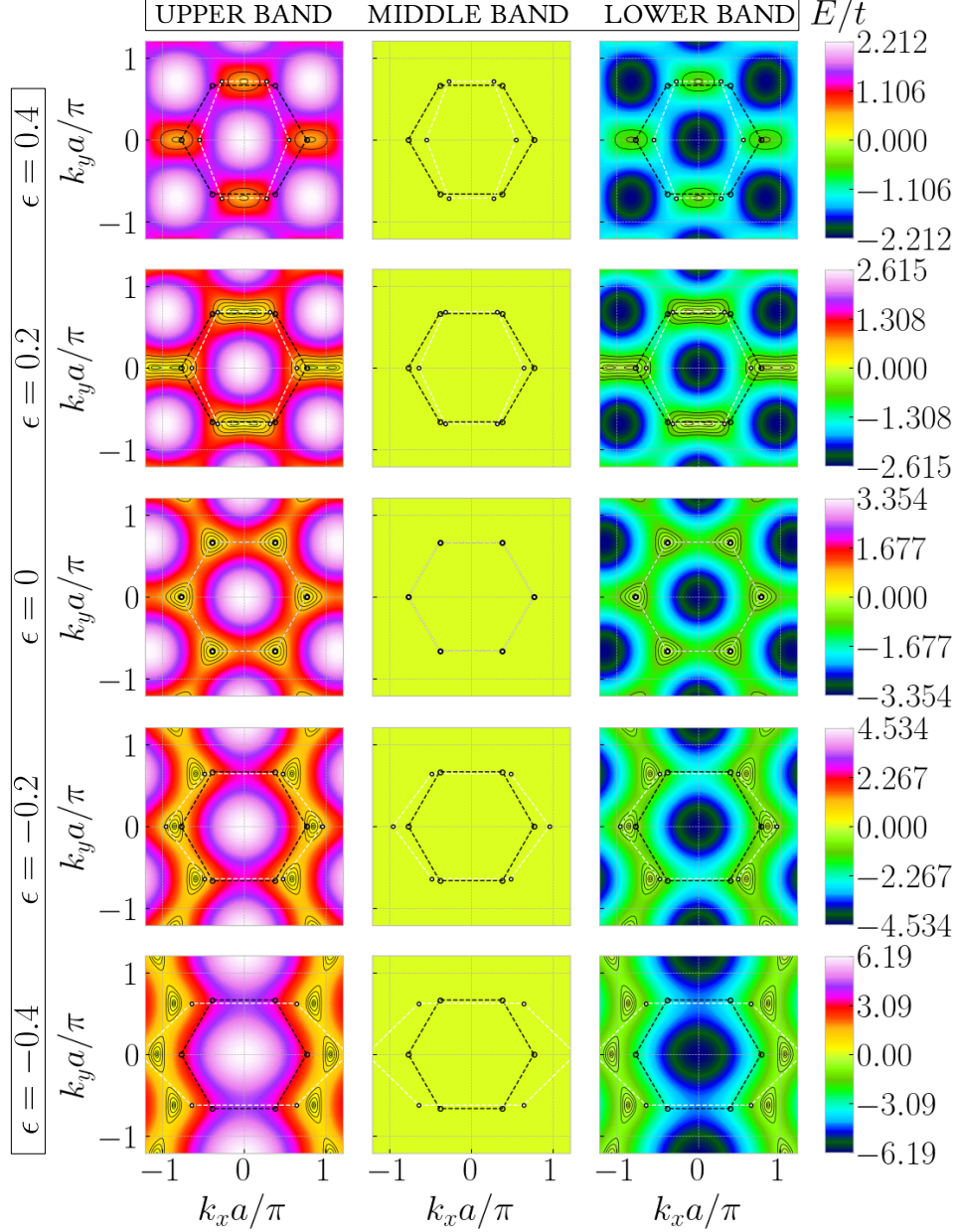
Figure 33 illustrates how each energy band of the $\alpha - T_3$ lattice is modified by UX strain for the strain amplitudes $\epsilon = 0.4$, $\epsilon = 0.2$, $\epsilon = 0$, $\epsilon = -0.2$, and $\epsilon = -0.4$. As anticipated, the flat band remains unaffected and electron-hole symmetry is preserved. In this situation, the applied strain can induce the opening of an energy gap in the spectrum, as shown in Fig. 29.

For this configuration, the effect of stretching the lattice is manifested in reciprocal space in an inverse fashion, as can be directly inferred from Eq. (4.13). In this case, we have $[(I + \bar{\epsilon})^{-1}]^T = (I + \bar{\epsilon})^{-1}$, *i.e.*, in the UX-strain case, the deformation in reciprocal space is governed by the inverse of the strain tensor applied in real space. An additional important consequence is that, since we are dealing with a uniform strain field, its effect in the Brillouin zone (BZ) is identical for all Dirac cones up to an overall sign. Furthermore, under strain, the strained-high-symmetry points $\mathbf{K}' = (I + \bar{\epsilon})^{-1}\mathbf{K}$ no longer coincide with the minima (maxima) of the conduction (valence) bands, which we will denote by $\mathbf{K}_D$ ⁴. A more detailed discussion of this behavior will be provided in the following sections.

Moreover, the constant-energy contours near the Fermi level [$E/t \approx 0$] in the vicinity of the Dirac cones exhibit a characteristic evolution. In the absence of strain, $\epsilon = 0$ [Fig. 33, columns 1 and 3, line 3], the constant-energy contours are circular, indicating an isotropic Fermi velocity. As strain is applied, these contours become elliptical, which in turn makes the Fermi velocity anisotropic. Another characteristic feature is that the influence of UX-strain on the band structure is asymmetric with respect to the sign of the strain amplitude ϵ , with more pronounced changes occurring under extension strain than under compression strain. For extensional strain, the valleys $\mathbf{K}_D$ and $\mathbf{K}'_D$ approach each

⁴ $\mathbf{K}_D$ denotes the vector associated with the positions of the minima (maxima) of the conduction (valence) band. In the absence of strain, it trivially follows that $\mathbf{K}_D = \mathbf{K}' = \mathbf{K}$, where $\mathbf{K}$ represents the corresponding high-symmetry point in the unstrained system.

Figure 33 – Contour plots of the lower (left panels), middle (central panels), and upper (right panels) energy bands of the $\alpha - T_3$ lattice with $\alpha = 0$ under UX strain for different strain amplitudes: $\epsilon = 0.4, 0.2, 0, -0.2, -0.4$ from top to bottom panels. The geometric contours superimposed on the plots correspond to the first unstressed (black dotted line) and strained (white dotted line) Brillouin zones, with the dots indicating high-symmetry points.

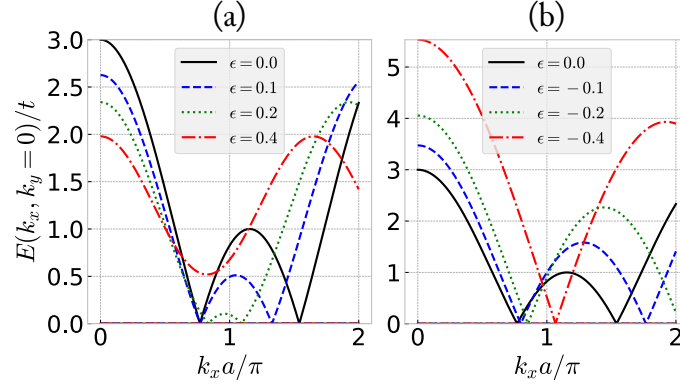


Source: The author.

other and eventually coalesce into a single point, while under compression strain, they move further apart.

Figure 34 displays the evolution of the dispersion relation of the $\alpha - T_3$ lattice with $\alpha = 0.5$ under UX strain along the k_x direction (with $k_y = 0$) for positive and negative values of strain amplitude ϵ . From these plots, the emergence of the gap in the band

Figure 34 – Dispersion relation of the $\alpha - T_3$ lattice with $\alpha = 0$ under UX strain along the k_x direction, with $k_y = 0$, for different strain amplitudes: $\epsilon = 0.0$ (black solid lines), $\epsilon = \pm 0.1$ (blue dashed lines), $\epsilon = \pm 0.2$ (green dotted lines), and $\epsilon = \pm 0.4$ (red dash-dotted lines), with the positive sign corresponding to the left panel (a) and the negative sign to the right panel (b).

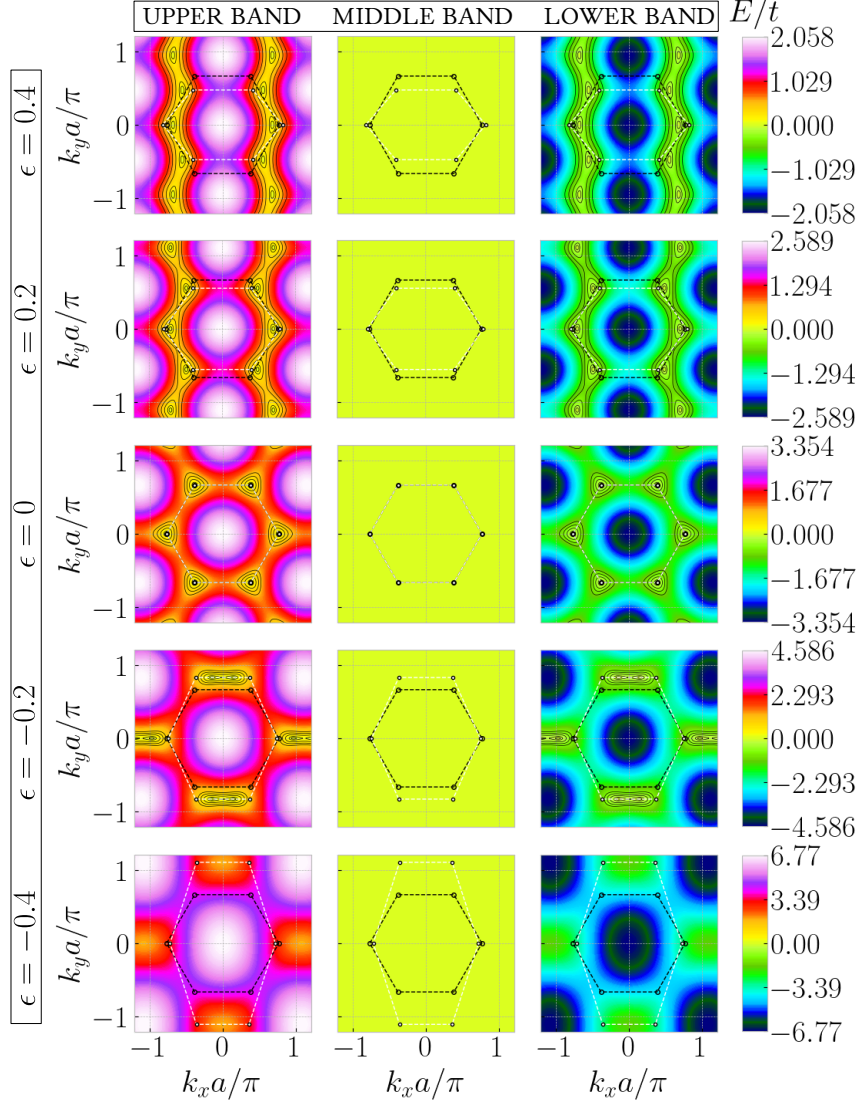


Source: The author.

structure becomes evident: it originates from the merging of two Dirac cones ($\mathbf{K}_D$ and $\mathbf{K}'_D$) (see Figure 34(a)), a phenomenon previously reported for graphene by Vitor M. Pereira and A. H. Castro Neto (PEREIRA *et al.*, 2009a). The case corresponding to UY-strain is presented in Fig. 35, which exhibits behavior qualitatively similar to that observed for UX-strain. In particular, several general features remain valid: the application of a strain tensor in real space induces an inverse deformation in reciprocal space, and the strained-high-symmetry points $\mathbf{K}' = (I + \bar{\epsilon})^{-1}\mathbf{K}$ under strain no longer coincide with the original Dirac point $\mathbf{K}_D$. Furthermore, the effect of UY-strain on the band structure is asymmetric with respect to the sign of the strain amplitude ϵ .

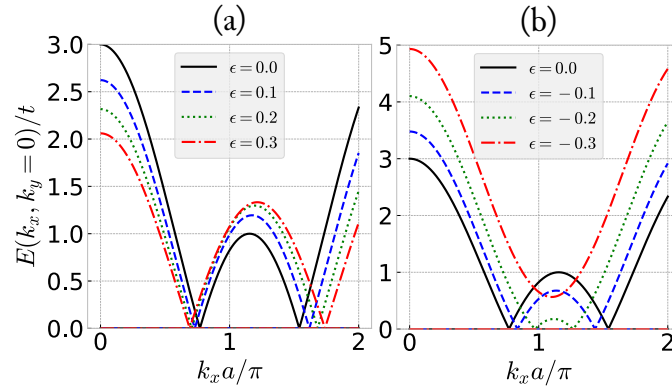
Under compression strain, the valleys located at $\mathbf{K}_D$ and $\mathbf{K}'_D$ move towards each other and eventually merge into a single point, see Fig. 36(a). In contrast, under extension strain, they move further apart (see Fig. 36(b)), in opposition to the trend found for UX-strain. In both cases, an energy gap opens in the band structure, but at different critical values of ϵ : whereas UX-strain produces a gap at $\epsilon = 0.23$, UY-strain leads to gap opening at $\epsilon = -0.23$. Moreover, the resulting energy gap grows more rapidly in the UY case. This behavior is evident from the isoenergy contours: for $\epsilon = -0.4$ [Fig. 35, columns 1 and 3, row 5], the corresponding isoenergies disappear, indicating the presence of a finite energy gap ($\Delta E/t > 0.8$). The BI strain configuration can be interpreted as the combined effect of the UX and UY strain cases. The resulting band-structure calculations indicate that its implementation in real space is mapped inversely into reciprocal space, as anticipated. However, in contrast to what is observed for the

Figure 35 – Same as Fig. 33, for UY-strain.



Source: The author.

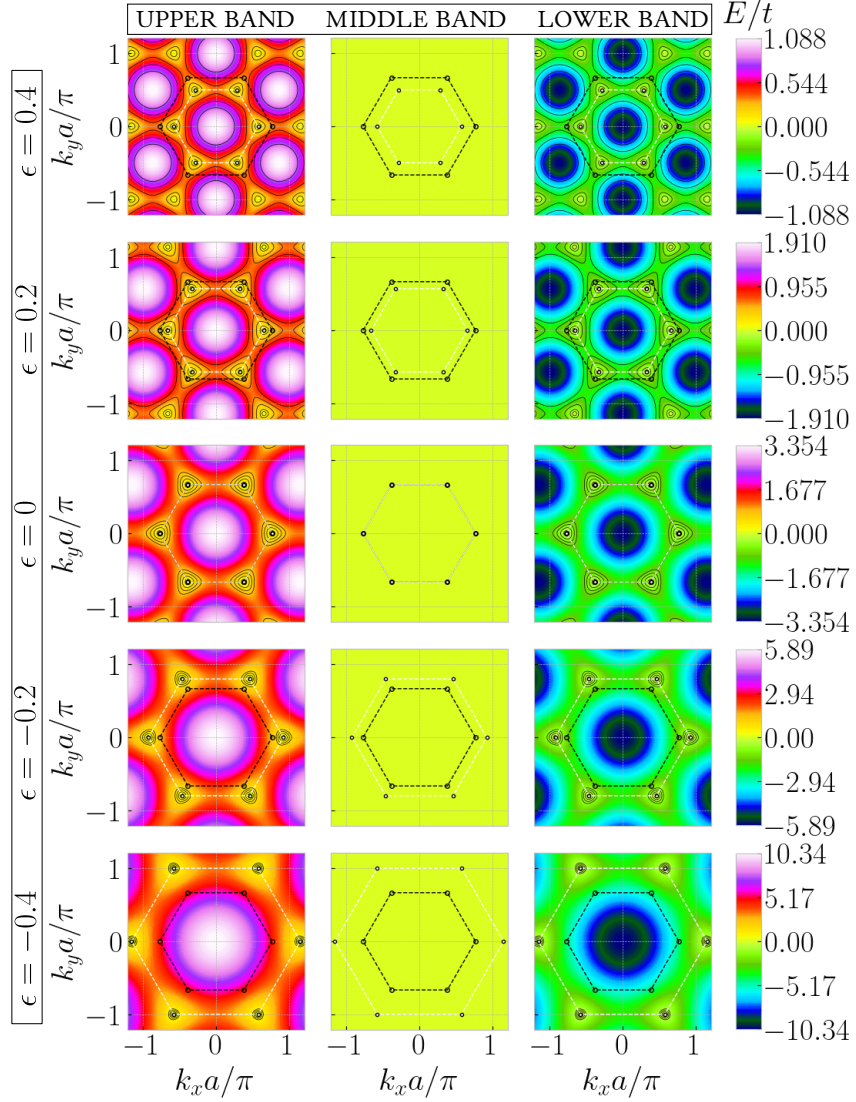
Figure 36 – Same as Fig. 34 for UY-strain.



Source: The author.

UX and UY cases, the strained high-symmetry points coincide with the conduction-band minima and valence-band maxima, such that $\mathbf{K}' = (I + \bar{\epsilon})^{-1}\mathbf{K} = \mathbf{K}_D$.

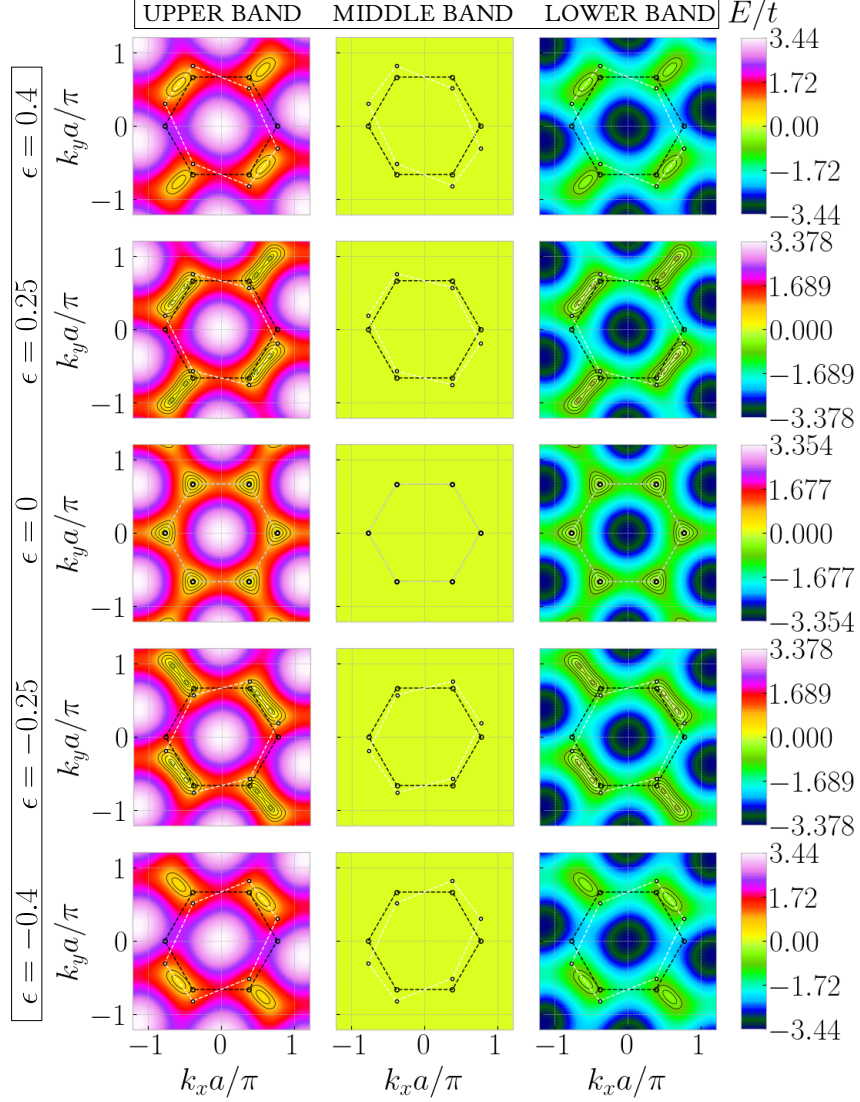
Figure 37 – Same as Fig. 33 for BI-strain.



Source: The author.

Moreover, this type of lattice deformation does not induce the opening of an energy gap in the electronic band structure, as shown in Fig. 29. This observation motivates a discussion regarding the possible connection between the absence of a band gap and the fact that the strained high-symmetry points coincide with the extrema of the conduction and valence bands. A further relevant feature is that this deformation preserves the isotropy, since the constant-energy contours in the vicinity of the Fermi level [$E/t \approx 0$] remain circular. In contrast to the axial strain configurations (UX, UY, and BI), the SX-type strain is symmetric with respect to the sign of the strain amplitude ϵ . More precisely, the deformed lattices corresponding to $\pm\epsilon$ are mirror images of each other, with the same absolute value of ϵ , as illustrated in Fig. 28(d). The associated energy spectra are likewise enantiomorphic. This behavior arises from the fact that the atomic

Figure 38 – Same as Fig. 33, but for the SX-strain field. Results are shown for different strain amplitudes, $\epsilon = 0.4, 0.25, 0, -0.25, -0.4$, ordered from the top to the bottom panels.

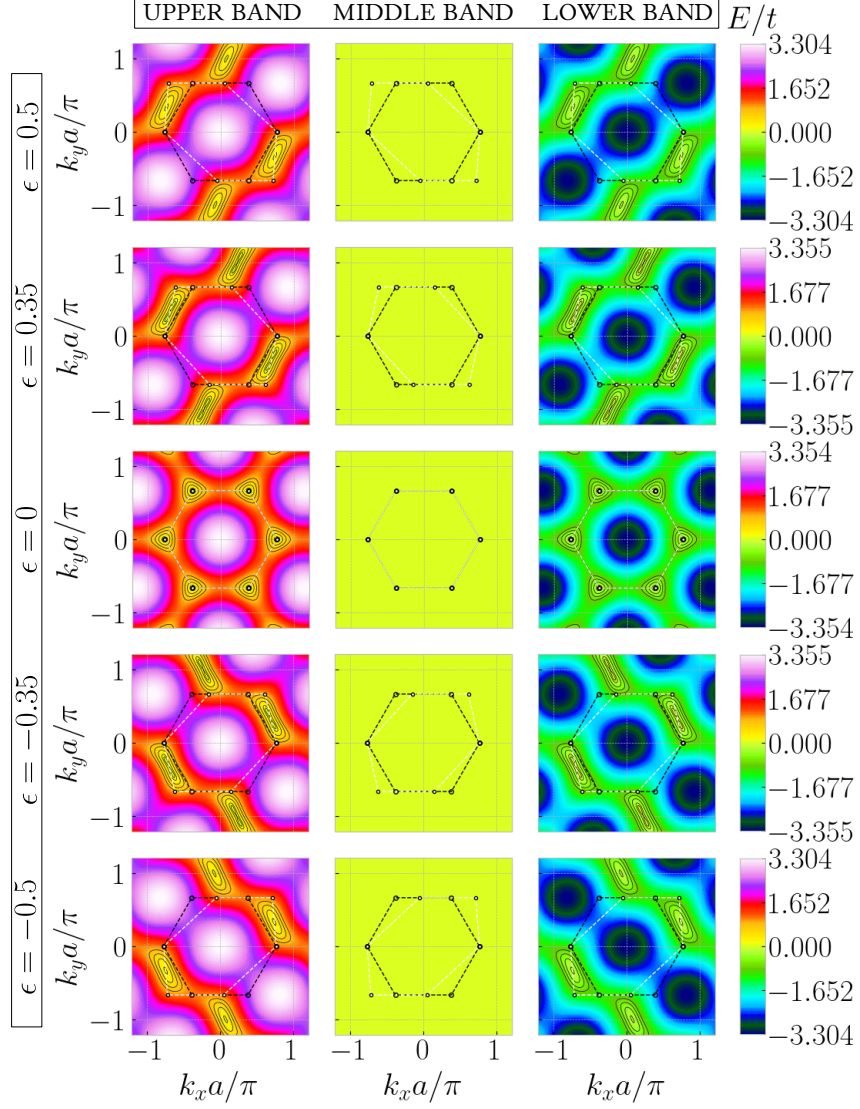


Source: The author.

displacements produced by a simple shear deformation are related by a mirror operation when comparing configurations generated by positive and negative values of ϵ . Formally, this symmetry can be expressed as $SX(\epsilon) = SX(-\epsilon)$.

In this case, the manner in which the strain acts in real space and is manifested in reciprocal space differs from that observed for the UX, UY, and BI strain configurations. For the SX-type deformation, its effect in reciprocal space can be identified with the negative of the SY-type strain acting in real space. To see this explicitly, let us consider Eq. (4.13), which in this case leads to the relation $[(I + \bar{\epsilon})_{SX}^{-1}]^T = -(I + \bar{\epsilon})_{SY}$. Another important consequence is that the strain-modified high-symmetry points $\mathbf{K}' = (I + \bar{\epsilon})^{-1}\mathbf{K}$

Figure 39 – Same as Fig. 33, but for the SY strain. Results are shown for different strain amplitudes, $\epsilon = 0.5, 0.35, 0, -0.35, -0.5$, from the top to the bottom panels.

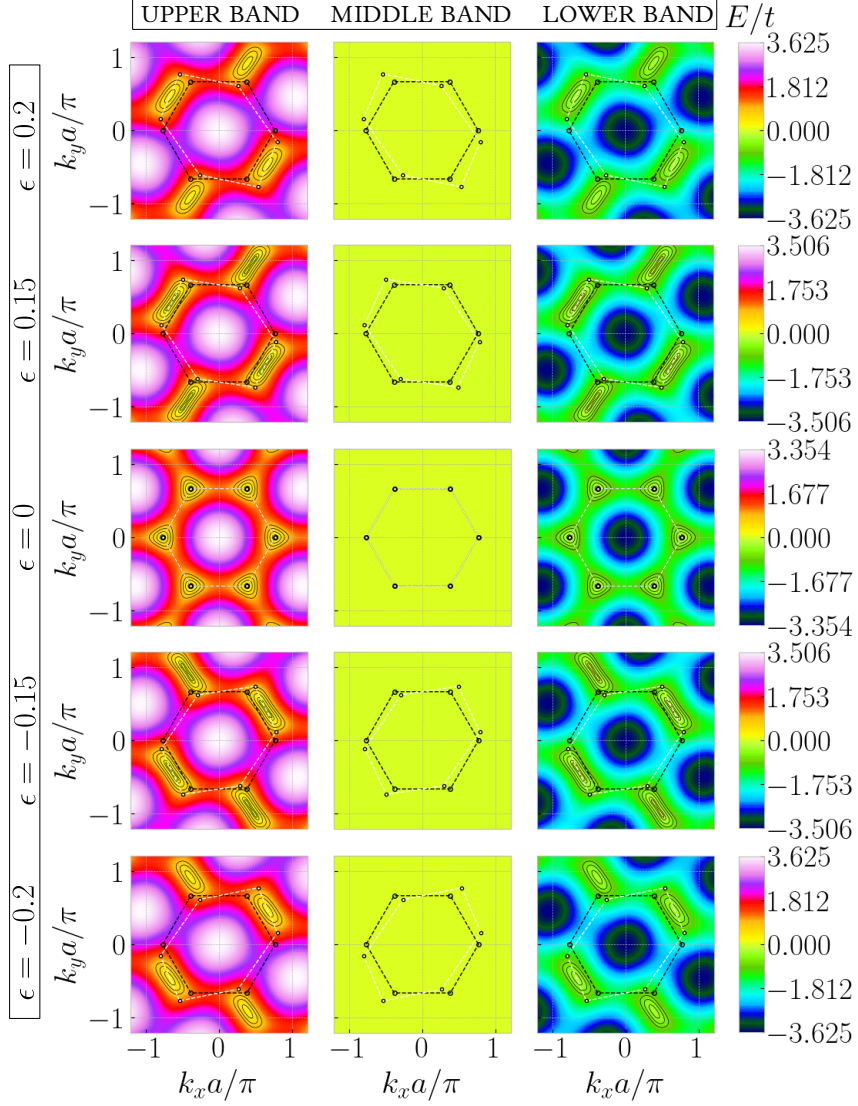


Source: The author.

no longer coincide with the original Dirac point $\mathbf{K}_D$. The strain thus induces anisotropy in the electronic bands in the vicinity of the Fermi level and, as in the other strain configurations, an energy gap opens when two inequivalent valleys ($\mathbf{K}_D$ and $\mathbf{K}'_D$) merge at a coalescent point.

As in the previous case, the same key features arise for SY-type strain: it is symmetric with respect to the sign of the strain amplitude ϵ , yielding an enantiomorphic spectrum. The strain-shifted high-symmetry points, $\mathbf{K}' = (I + \bar{\epsilon})^{-1}\mathbf{K}$, no longer coincide with the original Dirac point $\mathbf{K}_D$. This mismatch injects anisotropy into the electronic bands around the Fermi level and, as in other strain configurations, an energy gap opens when the two inequivalent valleys ($\mathbf{K}_D$ and $\mathbf{K}'_D$) coalesce at a single point. In particular,

Figure 40 – Same as Fig. 33 for PS-strain.



Source: The author.

the SY strain requires a larger strain amplitude than SX to open a gap (respectively, $\epsilon \approx \pm 0.39$ and $\epsilon \approx \pm 0.29$), and once opened, the gap increases more slowly under SY than under SX, so it may be identified by the isoenergy contours of Figs.38 and 39 in column 1.

The PS-strain corresponds to the combined effect of shear components in the xy plane (denoted SX and SY), and, analogously to other pseudo-shear configurations, it is symmetric with respect to the sign of the strain amplitude ϵ , thus giving rise to an enantiomorphic spectrum. The strain-shifted high-symmetry points, $\mathbf{K}' = (I + \bar{\epsilon})^{-1}\mathbf{K}$, no longer coincide with the original Dirac point $\mathbf{K}_D$. This mismatch introduces anisotropy into the electronic bands in the vicinity of the Fermi level and, as in other strain configurations, an energy gap emerges when the two inequivalent valleys ($\mathbf{K}_D$ and $\mathbf{K}'_D$) merge at a single point. In this particular case, the critical strain amplitude ϵ required for gap opening

is smaller ($\epsilon \approx 0.16$), and the corresponding gap-strain dependence exhibits a steeper increase.

In summary, the axial strain configurations UX, UY, and BI exhibit anti-symmetric behavior with respect to the sign of the strain amplitude, leading to distinct responses under extension and compression. Among these, the BI configuration is the only case that does not induce a gap in the electronic band structure and that preserves the isotropy of the energy dispersion in the vicinity of the Fermi level. In contrast, the UX and UY configurations give rise to strain-induced anisotropy, such that the deformed high-symmetry points in reciprocal space no longer coincide with the locations of the Dirac cones.

For the shear strain configurations SX, SY, and BI, the response is symmetric with respect to the sign of the strain amplitude. None of these shear cases preserves the isotropy of the bands near the Fermi level, and in all of them, the deformed high-symmetry points in reciprocal space are displaced relative to the Dirac cones. A detailed explanation of the strain-induced displacement (“drift”) of the Dirac cones away from the high-symmetry points will be provided in the following section.

4.4.3 *Strain-Induced Pseudomagnetic Fields in the $\alpha - T_3$ Lattice*

As previously discussed, the $\alpha - T_3$ lattice preserves the essential characteristics of graphene. This follows from the fact that the valence and conduction bands of these lattices are identical up to a multiplicative factor, while the additional band that emerges in the $\alpha - T_3$ lattice remains completely inert under deformation effects within a nearest-neighbor TB model in which all lattice sites are composed of the same atomic species; see Eqs. (4.29) and (4.30). Figures 33, 35, 37, 38, 39, and 40 illustrate the modifications of the energy bands and of the high-symmetry points in the Brillouin zone for the six types of strain applied to our system.

This systematic analysis raises the question of whether, under deformation, the positions of the high-symmetry points continue to coincide with the minima (maxima) of the conduction (valence) band, as they do in the undeformed case. Our results indicate that, in general, high-symmetry points in the strained lattice no longer satisfy this condition, with the sole exception of the BI deformation. Combined with the fact that the BI deformation is the only one that does not induce a band gap in the spectrum, this observation provides

a possible route to answering the aforementioned question.

In the absence of gap opening, we instead determine the values of $\mathbf{K}_D$, defined in this dissertation as the Dirac points, which satisfy $E(\mathbf{K}_D) = 0$. From Appendix A, we know that this condition is fulfilled when

$$\sum_{n=1}^3 t_n e^{-i[(I+\bar{\epsilon})^T \mathbf{K}_D] \cdot \mathbf{d}_n} = 0 \quad (4.64)$$

For the case of BI deformation, the hopping parameters take the form $t_n = t_0 e^{-\beta \epsilon_{xx}}$. Substituting this expression into Eq. (4.64), we obtain the following complex equation:

$$e^{-\frac{3}{2}iaK_{Dy}(\epsilon_{yy}+1)} + \cos[\sqrt{3}K_{Dx}(\epsilon_{xx}+1)] = 0. \quad (4.65)$$

Solving Eq. (4.65) yields

$$\mathbf{K}_D = \left(\mp \frac{m\pi}{\sqrt{3}a(\epsilon_{xx}+1)}, \frac{2n\pi}{3a(\epsilon_{yy}+1)} \right)^T, \quad \text{with } m \neq n = 0, 1, 2, \dots \quad (4.66)$$

which can be rewritten in terms of the high-symmetry points in the undeformed lattice, $\mathbf{K}$, as

$$\mathbf{K}_D = [(I + \bar{\epsilon})^{-1}]^T \mathbf{K}. \quad (4.67)$$

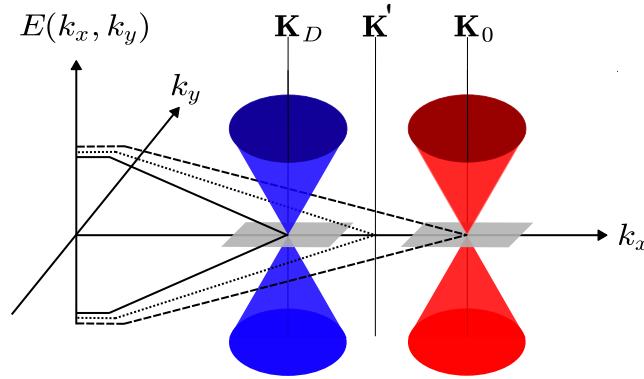
This result implies that, for this type of strain, the Dirac points coincide with the high-symmetry points of the strained reciprocal lattice (see Eq. (4.13)). Consequently, it not only supports the features already described for the BI deformation case but also provides additional insight into the behavior under other deformation types. In particular, it shows that the hopping amplitudes are directly related to both the energy gap, as established by the inequality (4.58), and to the positions of the high-symmetry points. Specifically, in a hypothetical situation where $t_1 = t_2 = t_3$, no gap opens, and the high-symmetry points coincide with the corners of the first deformed Brillouin zone.

For the uniaxial and shear deformation cases, the hopping parameters t_1 , t_2 , and t_3 become inequivalent, and the Dirac points $\mathbf{K}_D$ nevertheless persist according to the definition adopted here, namely, that $E(\mathbf{K}_D) = 0$ within certain intervals⁵. However, these Dirac points are displaced from the high-symmetry points in the strained Brillouin zone, given by $\mathbf{K}' = [(I + \bar{\epsilon})^{-1}]^T \mathbf{K}_0$. This behavior had previously been reported for graphene under uniaxial strain (PEREIRA *et al.*, 2009a) and has been further confirmed and

⁵ The condition $E(\mathbf{K}_D) = 0$ remains valid as long as no band gap opens, which motivates the reference to defined intervals; see Fig. 29.

generalized in this dissertation for shear deformations. Figure 41 schematically illustrates the drift of the Dirac cone in the α - T_3 lattice induced by uniaxial strain applied along the x direction.

Figure 41 – Representation of the behavior of the Dirac cone under uniaxial tension in the x direction for the α - T_3 lattice. The real position of the Dirac cone under deformation is given by $\mathbf{K}_D$ which is different from the deformed high symmetry point in the reciprocal space $\mathbf{K}' = [(I + \bar{\epsilon})^{-1}]^T$ and $\mathbf{K}_0$ shows the initial position without strain.



Source: Figure adapted from reference (OLIVA-LEYVA; NAUMIS, 2015).

The position of the cone $\mathbf{K}_D$ generally does not coincide with that of the high-symmetry point in the deformed reciprocal space, denoted by $\mathbf{K}'$, except in the special case of the BI deformation, for which $\mathbf{K}_D = \mathbf{K}'$. The new locations of the Dirac points in the general situation where t_1 , t_2 , and t_3 differ can be determined by solving the complex equation (4.64). This equation can be treated using perturbative methods.⁶ Within a second-order strain approximation, the positions of the Dirac cones for the general case are given by

$$\mathbf{G} = (I + \bar{\epsilon})^T \mathbf{K}_D = \mathbf{K}_0 + \mathbf{A}^{(1)} + \mathbf{A}^{(2)} + O(\epsilon^3), \quad (4.68)$$

where $\mathbf{A}^{(j)}$ is referred to as the vector pseudopotential. Its first-order components are given by

$$A_x^{(1)} = \frac{\csc(K_{0x}a\sqrt{3}/2)}{a\sqrt{3}} \left[\Delta_1^{(1)} \operatorname{Re}(e^{-\frac{3}{2}iK_{0y}}) + (\Delta_2^{(1)} + \Delta_3^{(1)}) \operatorname{Re}(e^{-i\frac{\sqrt{3}}{2}aK_{0x}}) \right] \quad (4.69)$$

$$A_y^{(1)} = \frac{1}{a[\operatorname{Re}(e^{-\frac{3}{2}iK_{0y}}) - \cos(K_{0x}a\sqrt{3}/2)]} \left[(\Delta_2^{(1)} - \Delta_3^{(1)}) \operatorname{Im}(e^{-i\frac{\sqrt{3}}{2}aK_{0x}}) \right]. \quad (4.70)$$

⁶ The complete derivation is presented in Appendix A.

In the second order, the components read

$$A_x^{(2)} = \frac{\csc(K_{0x}a\sqrt{3}/2)}{a\sqrt{3}} \sum_{n=1}^3 \operatorname{Re}(e^{-i\mathbf{K}_0 \cdot \mathbf{d}_n}) \left[\Delta_n^{(2)} + \frac{(\mathbf{A}^{(1)} \cdot \mathbf{d}_n)^2}{2} \right] + \operatorname{Im}(e^{-i\mathbf{K}_0 \cdot \mathbf{d}_n}) \left[\Delta_n^{(1)} \mathbf{A}^{(1)} \cdot \mathbf{d}_n \right] \quad (4.71)$$

$$A_y^{(2)} = \frac{1}{a[\operatorname{Re}(e^{-\frac{3}{2}iK_{0y}}) - \cos(K_{0x}a\sqrt{3}/2)]} \sum_{n=1}^3 -\operatorname{Re}(e^{-i\mathbf{K}_0 \cdot \mathbf{d}_n}) \left[\Delta_n^{(1)} \mathbf{A}^{(1)} \cdot \mathbf{d}_n \right] + \operatorname{Im}(e^{-i\mathbf{K}_0 \cdot \mathbf{d}_n}) \left[\Delta_n^{(2)} + \frac{(\mathbf{A}^{(1)} \cdot \mathbf{d}_n)^2}{2} \right]. \quad (4.72)$$

Non-uniform strain fields in Dirac and Weyl materials give rise to effective pseudomagnetic fields (LIU; LU, 2022; SUN *et al.*, 2022; LIU, 2020). These effective fields are defined through the standard relation $\mathbf{B} = \nabla \times \mathbf{A}$. In this dissertation, however, we restrict our analysis to uniform strain configurations, which by definition cannot generate pseudomagnetic fields, since in this case $\mathbf{B} = \nabla \times \mathbf{A} = 0$. The term “vector pseudopotential” is therefore employed here primarily to emphasize the formal analogy with the electromagnetic gauge potential, despite the absence of an associated (pseudo)magnetic field under uniform strain.

The vector pseudopotentials given by Eqs. (4.69), (4.70), (4.71) and (4.72) are valid for a generic high symmetry point $\mathbf{K}_0 = (K_{0x}, K_{0y})$, in addition the terms $\Delta_n^{(1)}$ and $\Delta_n^{(2)}$ correspond, respectively, to first and second order in strain percent approximations for the hopping t'_n and are given by

$$\Delta_n^{(1)} = -\frac{\beta}{a^2} \mathbf{d}_n \cdot \bar{\epsilon} \mathbf{d}_n, \quad (4.73)$$

$$\Delta_n^{(2)} = -\frac{\beta}{2a^2} |\bar{\epsilon} \mathbf{d}_n|^2 + \frac{\beta(\beta+1)}{2a^4} (\mathbf{d}_n \cdot \bar{\epsilon} \mathbf{d}_n)^2. \quad (4.74)$$

To explore some properties of pseudopotentials, let us consider the particular case in which $\mathbf{K}_0 = (4\pi/(3\sqrt{3}a), 0)$ and the simple shear terms are the same in the xy directions ($\epsilon_{xy} = \epsilon_{yx}$), thus

$$A_x^{(1)} = \frac{\beta(\epsilon_{xx} - \epsilon_{yy})}{2a} \quad (4.75)$$

$$A_y^{(1)} = \frac{-\beta\epsilon_{xy}}{a}. \quad (4.76)$$

$$A_x^{(2)} = \frac{\beta(4\beta+1)[(\epsilon_{xx} - \epsilon_{yy})^2 - 4\epsilon_{xy}^2]}{16a} \quad (4.77)$$

$$A_y^{(2)} = \frac{\beta(4\beta + 1)(\epsilon_{xx} - \epsilon_{yy})\epsilon_{xy}}{4a}. \quad (4.78)$$

The results we obtained agree with those of Oliva-Leyva e Wang (2017) for first-order terms and for second-order cases. For other high-symmetry points, the values are the same, minus a global signal. If we consider a strain of type BI, we can notice that the pseudopotentials are zero, which causes Eq.(4.68) to reduce to Eq.(4.67), as expected.

The terms governing the displacement of Dirac cones away from high-symmetry points are relevant in the context of non-uniform deformations, since they do not directly determine the gauge associated with the pseudomagnetic field induced by such deformations. To illustrate this, consider a non-uniform uniaxial strain field of the form $\mathbf{u} = (0, \frac{c}{2\beta}y^2)$. The components of the strain tensor (pseudopotential) are defined as $\epsilon_{ij} = (\partial_i u_j + \partial_j u_i)/2$ for $i, j = x, y$. For this specific deformation, the nonvanishing components are

$$\epsilon_{xx} = 0, \quad \epsilon_{yy} = \frac{c}{\beta}y, \quad (4.79)$$

and the corresponding first-order pseudovector potential ($\mathbf{A}^{(1)}$) assumes the gauge

$$(A_x, A_y) = \left(\frac{c}{2a}y, 0 \right), \quad (4.80)$$

which gives rise to the effective pseudomagnetic field

$$\mathbf{B} = \frac{c}{2a}\hat{z}. \quad (4.81)$$

This type of non-uniform deformation is typically implemented in graphene and related nanoribbon structures. For a more detailed discussion, see Refs. (SUN *et al.*, 2022; FILUSCH *et al.*, 2021; SUN *et al.*, 2023; OLIVA-LEYVA; WANG, 2017).

4.5 Strain in nanoribbons of $\alpha - T_3$

As previously discussed, the application of strain to the “infinite” system modifies both the primitive lattice vectors and the hopping amplitudes between atomic sites, in accordance with Eqs. (4.1) and (4.9). The results indicate that, within the nearest-neighbor TB approximation for the $\alpha - T_3$ lattice, the third site, controlled by the morphological parameter responsible for the emergence of the flat band, does not introduce substantial deviations from the graphene limit. In fact, all physical quantities obtained in this regime can be expressed as $(\sqrt{\alpha^2 + 1}) \times \text{graphene}$.

In contrast, when considering finite-width geometries, *e.g.*, nanoribbons, the behavior changes significantly. For nanoribbons with zigzag edge terminations in the transition regime of the $\alpha - T_3$ lattice, the system exhibits semiconducting characteristics, in stark contrast to graphene zigzag nanoribbons, which remain metallic under analogous conditions (WAKABAYASHI *et al.*, 2010).

Motivated by this distinction, we now investigate the effect of strain on confined $\alpha - T_3$ systems and analyze the resulting electronic properties. The implementation of strain follows the same procedure adopted for the infinite lattice. The matrix elements defining the TB Hamiltonian for nanoribbons with zigzag ($Z\alpha - T_3$ NRs) and armchair ($A\alpha - T_3$ NRs) edge terminations under strain are summarized in the table below.

Table 10 – Element matrices for each type of nanoribbon edge with strain.

Element	Zigzag AA/AB/AC	Armchair
$\gamma^{AB}(t')$	$t' \cos \theta e^{i\mathbf{k} \cdot \mathbf{d}'_1}$	$t' \cos \theta e^{-i\mathbf{k} \cdot \mathbf{d}'_1}$
$\eta^{AB}(t')$	$t' \cos \theta (e^{i\mathbf{k} \cdot \mathbf{d}'_2} + e^{i\mathbf{k} \cdot \mathbf{d}'_3})$	$t' \cos \theta e^{-i\mathbf{k} \cdot \mathbf{d}'_2}$
$\lambda^{AB}(t')$	0	$t' \cos \theta e^{-i\mathbf{k} \cdot \mathbf{d}'_3}$
$\gamma^{AC}(t'_A)$	$t'_A \sin \theta (e^{-i\mathbf{k} \cdot \mathbf{d}'_2} + e^{-i\mathbf{k} \cdot \mathbf{d}'_3})$	$t'_A \sin \theta e^{i\mathbf{k} \cdot \mathbf{d}'_3}$
$\eta^{AC}(t'_A)$	$t'_A \sin \theta e^{-i\mathbf{k} \cdot \mathbf{d}'_1}$	$t'_A \sin \theta e^{i\mathbf{k} \cdot \mathbf{d}'_2}$
$\lambda^{AC}(t'_A)$	0	$t'_A \sin \theta e^{i\mathbf{k} \cdot \mathbf{d}'_1}$
$\gamma^{BC}(t'_B)$	$t'_B \sin \theta e^{i\mathbf{k} \cdot \mathbf{d}'_1}$	$t'_B \sin \theta e^{-i\mathbf{k} \cdot \mathbf{d}'_1}$
$\eta^{BC}(t'_B)$	$t'_B \sin \theta (e^{i\mathbf{k} \cdot \mathbf{d}'_2} + e^{i\mathbf{k} \cdot \mathbf{d}'_3})$	$t'_B \sin \theta e^{-i\mathbf{k} \cdot \mathbf{d}'_2}$
$\lambda^{BC}(t'_B)$	0	$t'_B \sin \theta e^{-i\mathbf{k} \cdot \mathbf{d}'_3}$

In strain theory, the defining feature of shear strains is the preservation of the volume of the deformed solid, since the determinant of the corresponding transformation matrix equals unity (see Eq. (4.4)). This property is particularly relevant in the context of deformations in confined systems, such as nanoribbons, whose structural and electronic characteristics exhibit strong width dependence. Consequently, in this section, we restrict the application of shear strain to the periodic direction, thereby preserving the effective thickness of the nanoribbons.

The geometric components listed in Table 10 are transformed according to

$$\begin{pmatrix} r'_x \\ r'_y \end{pmatrix} = \begin{pmatrix} 1 & \epsilon_{xy} \\ 0 & 1 \end{pmatrix} \begin{pmatrix} r_x \\ r_y \end{pmatrix}, \quad (4.82)$$

where the corresponding hopping parameters are specified in Eq. (4.9). Since graphene is included as a particular case in our analysis, we follow the methodology of Bandeira *et al.*

(2020), who investigated graphene nanoribbons under simple shear strain and an external electric field. In that work, the shear strain was parameterized in terms of a dimensionless percentage $\gamma(\%)^7$, defined according to the edge termination as

$$\gamma = \epsilon_{xy}/\sqrt{3}, \quad \text{zigzag edge}, \quad (4.83)$$

$$\gamma = \epsilon_{xy}\sqrt{3}, \quad \text{armchair edge}. \quad (4.84)$$

As previously discussed, the application of shear strain satisfies the symmetry property $\text{SX}(\epsilon) = \text{SX}(-\epsilon)$, see Fig. 38. Therefore, in what follows, we restrict our analysis to the case of positive shear strain, with a maximum applied deformation of $\gamma = 20\%$.

4.5.1 Results for zigzag case

Figure 42 shows that the dispersion relation in the vicinity of the Fermi level is modified for the three cases $N = 20$, $N = 21$, and $N = 22$ upon application of shear strain along the periodic direction. A general feature of the effect of simple shear applied along the periodic direction in $Z\alpha - T_3\text{NRs}$ for the two types of terminations, t_A and t_B , is the lifting of the degeneracy at $k = \frac{\pi}{a\sqrt{3}}$.

In Figs. 44, we present contour plots of the band gap as a function of the lattice morphology and strain amplitude γ .

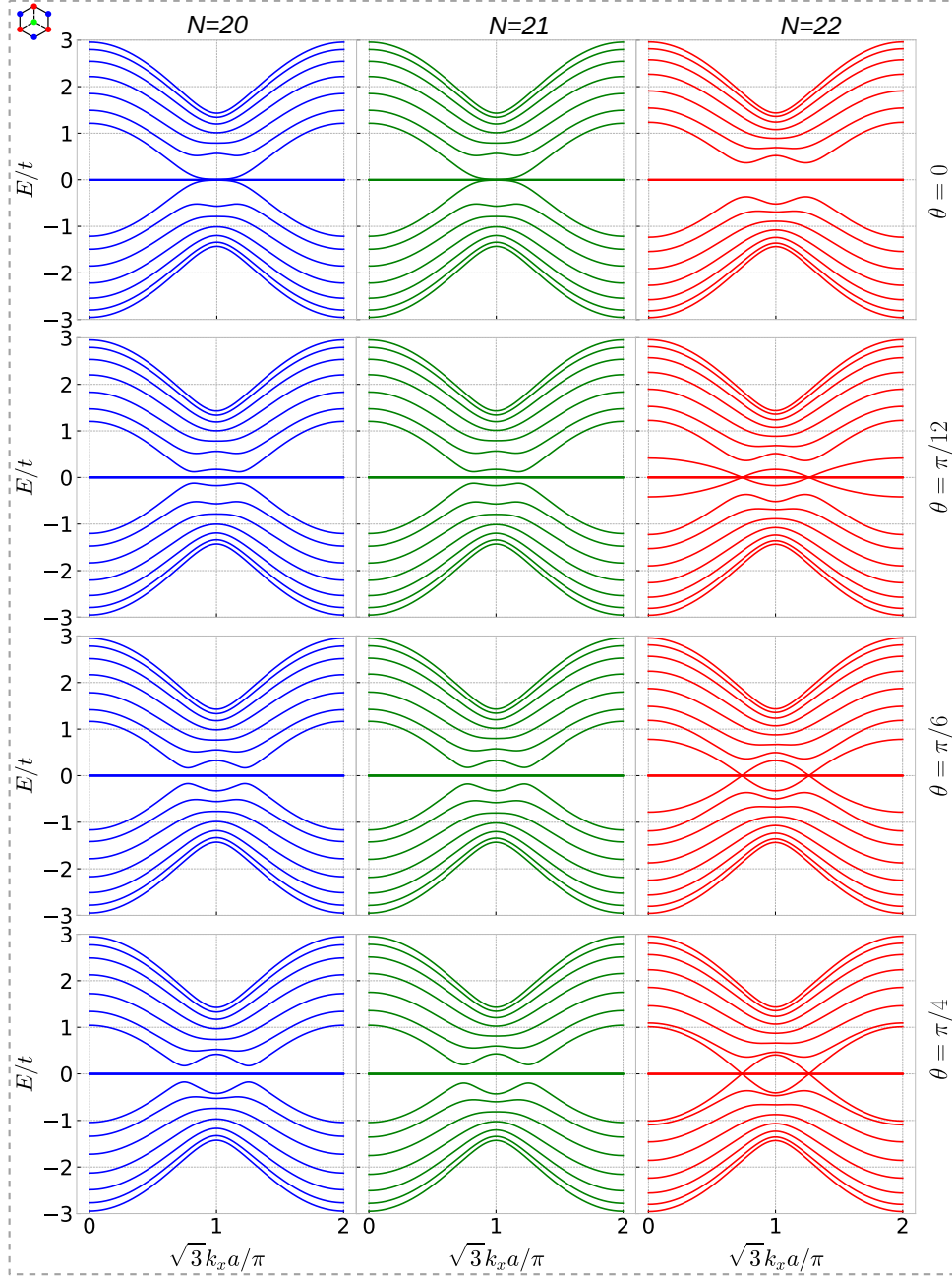
The $3p$ and $3p + 2$ families exhibit identical behavior irrespective of the type of bond between the central site and the HCL sites and display similar trends with respect to strain amplitude and morphological angle. In contrast, the $3p + 1$ families differ: the t_A -type termination leads to a metallic (conducting) system, whereas the t_B -type termination yields a semiconducting system, both showing only a weak dependence on mechanical deformation and lattice morphology.

4.5.2 Results for armchair case

The dispersion relation for the armchair nanoribbon is organized into three distinct families, classified according to the number of atomic lines across the ribbon width, W . These families exhibit semiconducting behavior for $W = 3p$ and $W = 3p + 1$, and metallic behavior for $W = 3p + 2$, where $p = 1, 2, 3, \dots$. Consequently, the results obtained for specific ribbon widths can be systematically generalized within each family.

⁷ This percentage is unrelated to any matrix element associated with the nanoribbons; it is merely a

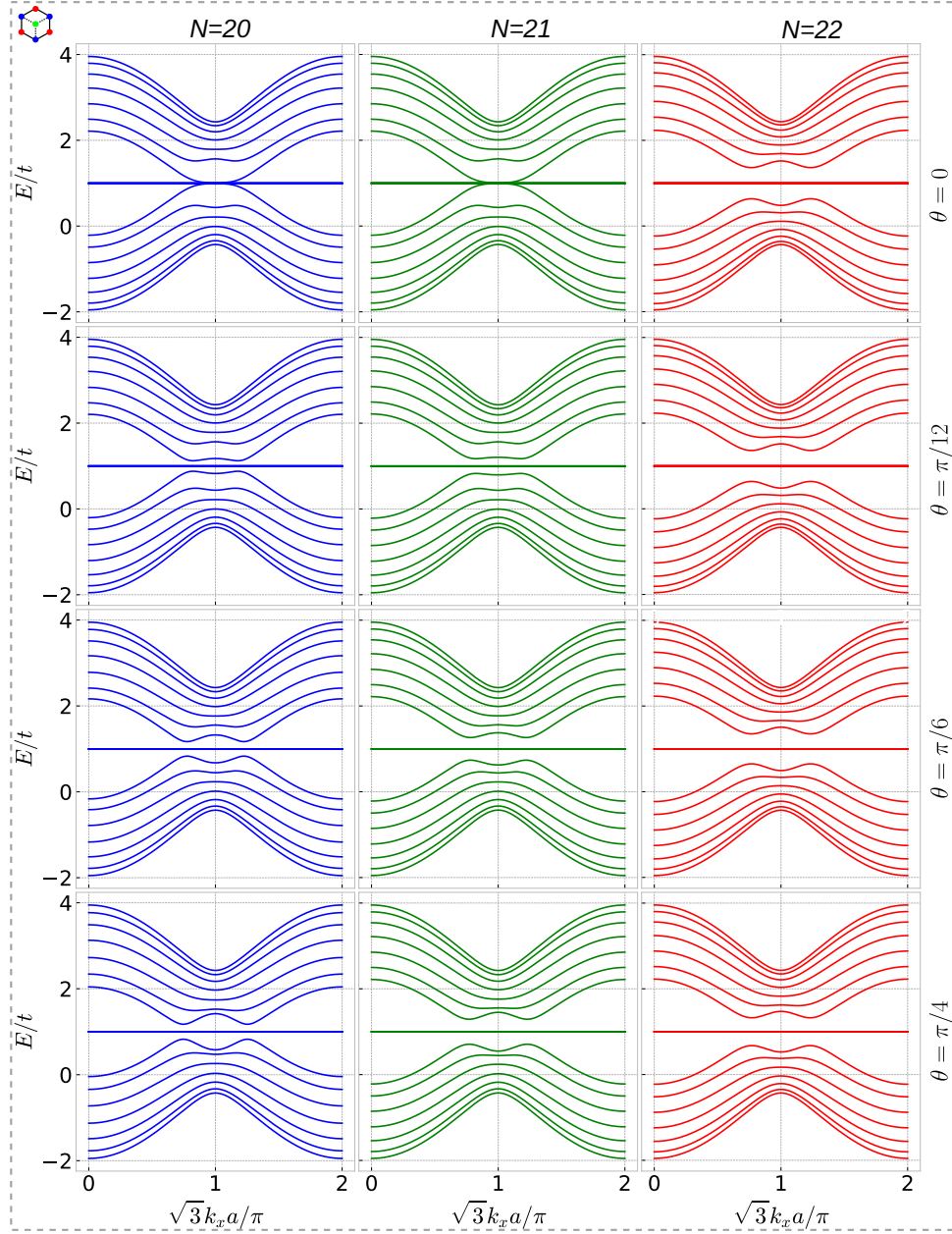
Figure 42 – Band structures for zigzag $\alpha - T_3$ nanoribbons with different terminations, with simple shear strain ($\gamma = 10\%$) applied along the periodic direction and morphological angle $\theta = \tan^{-1} \alpha$: $\theta = 0$, $\theta = \pi/12$, $\theta = \pi/6$, and $\theta = \pi/4$.



Source: The author.

Figure 45 shows that the dispersion relation in the vicinity of the Fermi level is modified for the three cases $N = 20$, $N = 21$, and $N = 22$ upon application of shear strain along the periodic direction. For $N = 20$, an energy bandgap emerges for the transition configurations $0 < \theta \leq \pi/4$, which are metallic in the absence of strain. For the other two cases, $N = 21$ and $N = 22$, which already exhibit a finite bandgap, shear strain induces a

convenient measure of the applied shear strain.

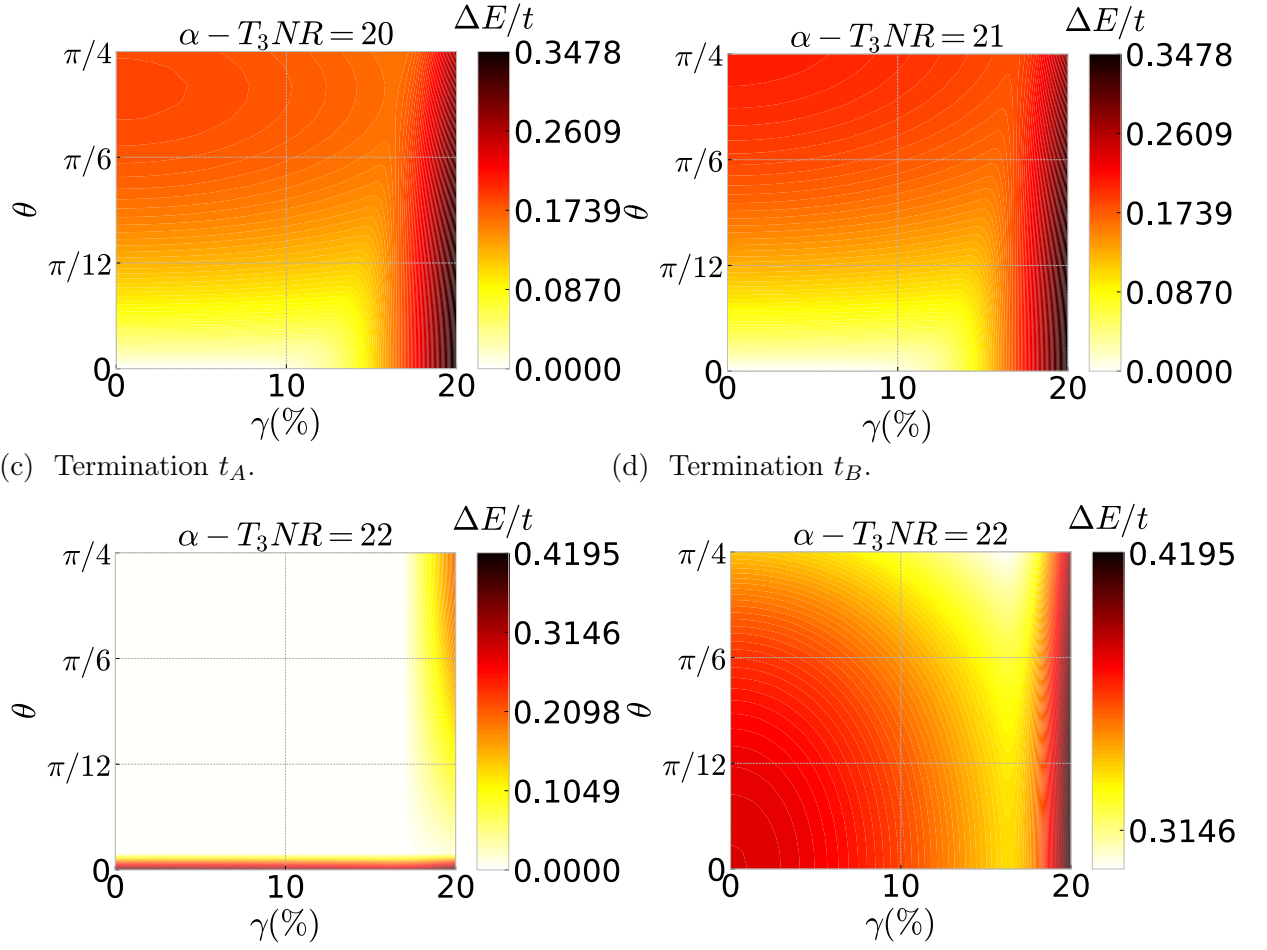
Figure 43 – Same as Fig. 42, but for the t_B termination.

Source: The author.

slight increase in the gap magnitude and a displacement of the bands in momentum space. The corresponding behavior of the bandgap as a function of the lattice morphology and strain amplitude γ (considered up to 20% in this dissertation) is presented in the contour plots below.

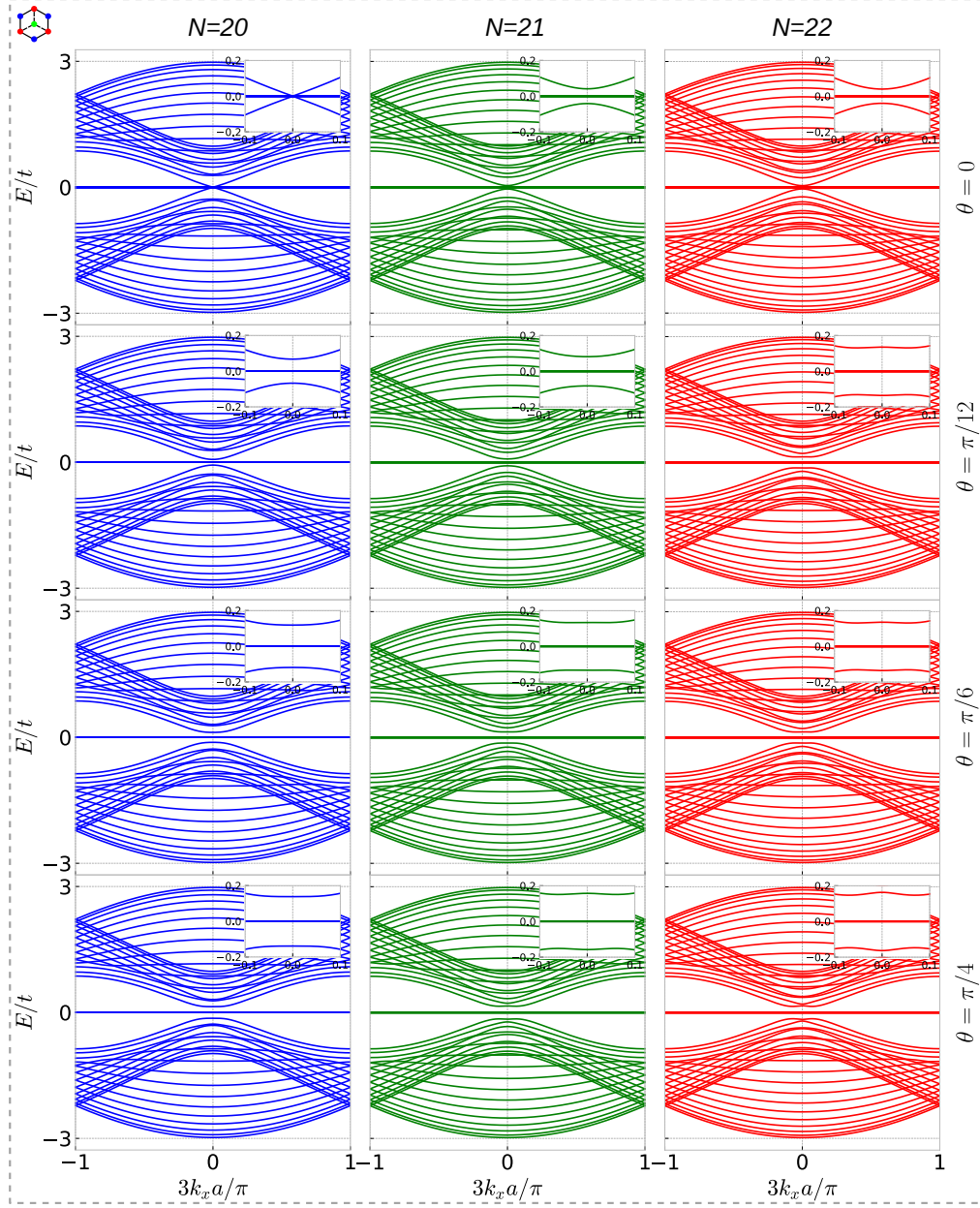
From these results, it is evident that the three families $3p$, $3p + 1$, and $3p + 2$ undergo modifications in their dispersion relations near the Fermi level under shear strain. The most pronounced effect occurs for the $3p + 2$ family (see Fig. 46a), which undergoes a transition from metallic to semiconducting behavior upon the application of strain. In

Figure 44 – Contour plots of the energy gap of $Z\alpha - T_3NR$ s as a function of the strain amplitude and morphological angle θ : $0, \pi/12, \pi/6$, and $\pi/4$.
 (a) Termination t_A or t_B . (b) Termination t_A or t_B .

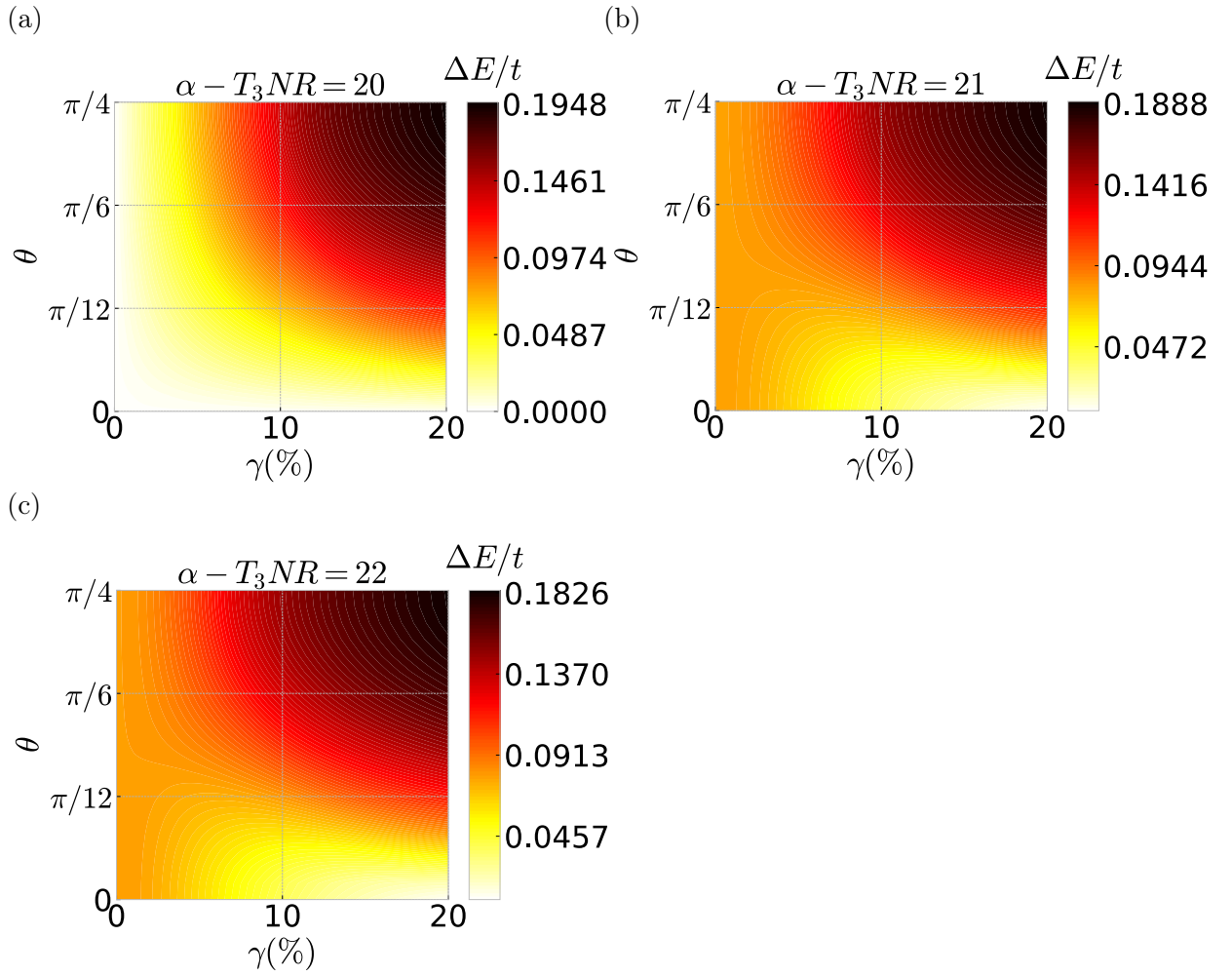


Source: The author.

addition, for all three families, the bandgap magnitude can be continuously tuned by increasing the strain amplitude γ .

Figure 45 – Same as Fig. 42 for $A\alpha - T_3$ NRs.

Source: The author.

Figure 46 – Same as Fig. 42 for $A\alpha - T_3NR$ s.

Source: The author.

5 CONCLUSIONS AND FUTURE WORK

Motivated by the distinctive morphological characteristics of the $\alpha - T_3$ lattice and by finite-size quantum effects already observed in one of its limiting cases (graphene), we employ a tight-binding framework to systematically examine how the electronic properties of the $\alpha - T_3$ lattice and its nanoribbons are modified by both intrinsic and extrinsic parameters. As intrinsic parameters, we consider the morphological angle α , the distinct coupling configurations between the HCL and the central site, and the various possible edge terminations. As extrinsic parameters, we investigate the influence of uniform in-plane deformation fields.

In Chapter 2, we analyze the infinite lattice using the tight-binding model in two complementary formalisms: (i) first quantization, via Bloch functions, and (ii) second quantization, via creation and annihilation operators. We study the resulting electronic spectrum for the two inequivalent coupling schemes between the central site and the HCL and find that, within the orthogonal tight-binding approximation, in which all atomic sites share the same onsite energy, these different coupling configurations do not alter the band structure. Within the continuum limit, we show how the lattice morphology enables a continuous interpolation between Dirac quasiparticles with effective pseudospin $S = 1/2$ and Dirac quasiparticles with effective pseudospin $S = 1$.

In Chapter 3, we examine the quasi-one-dimensional confinement using the tight-binding model in the second-quantization formalism and the Heisenberg equation of motion in order to analyze how the electronic states of $\alpha - T_3$ nanoribbons are affected by morphology, edge termination, and thickness. The $Z\alpha - T_3$ NRs nanoribbons exhibit morphology-dependent electronic characteristics, with the graphene limit representing a special case that differs qualitatively from the others. The intermediate morphologies can be grouped into three distinct families according to the number of atomic chains, $N = 3p$ (semiconducting), $N = 3p + 1$ (semiconducting), and $N = 3p + 2$ (metallic or semiconducting), where $p = 1, 2, 3, \dots$. In particular, the coupling between the HCL and the central C site is responsible for driving the $N = 3p + 2$ family from a metallic to a semiconducting regime, or vice versa. In contrast, the $A\alpha - T_3$ NRs nanoribbons are insensitive to morphology in this respect, exhibiting the same dispersion relation as graphene apart from the presence of a flat band. They are likewise classified into three families by the number of atomic chains, $N = 3p$ (semiconducting), $N = 3p + 1$

(semiconducting), and $N = 3p + 2$ (metallic), with $p = 1, 2, 3, \dots$

In Chapter 4, starting from a tight-binding Hamiltonian combined with continuum elasticity theory for two-dimensional materials, we undertake a systematic analysis of six distinct classes of in-plane deformations in the $\alpha - T_3$ lattice: uniaxial strain along the x and y directions, biaxial strain, simple shear along the x and y directions, and pure shear. We show that biaxial strain is the only deformation that does not induce the opening of a band gap in the electronic spectrum. For all other deformation types, we derive closed-form analytical expressions characterizing the evolution of the energy gap as a function of the strain parameters. In addition, we analyze the displacement of the Dirac cones from high-symmetry points in the Brillouin zone and clarify their relation to emergent pseudo-magnetic fields arising in the presence of non-uniform strain. We further apply shear strain along the periodic direction of $\alpha - T_3$ nanoribbons and demonstrate that, for nanoribbons with zigzag edge termination, the electronic properties exhibit only a weak dependence on both strain and edge morphology. In contrast, for armchair-terminated nanoribbons, the band-gap magnitude can be continuously tuned by increasing the shear strain amplitude.

As future extensions of this work, we intend to incorporate external perpendicular electric and magnetic fields, as well as spatially non-uniform deformation fields, with the aim of elucidating the differences between Landau levels generated by real magnetic fields and those induced by strain-related pseudo-magnetic fields, and to determine how both sets of Landau levels are modified by an external electric field.

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APPENDIX A – INVESTIGATION OF THE DIRAC POINTS OF THE $\alpha - T_3$ LATTICE UNDER STRAIN

To investigate what happens to the Dirac points of the $\alpha - T_3$ lattice under strain, we will base ourselves on the work done by Oliva-Leyva e Wang (2017) for the graphene.

The eigenvalues of the $\alpha - T_3$ lattice under strain are given by:

$$\lambda(\mathbf{k}) = E \quad \text{and} \quad \lambda_{\pm}(\mathbf{k}) = E \mp |f(\mathbf{k})| \sqrt{\alpha^2 + 1}, \quad (\text{A.1})$$

where

$$f(\mathbf{k}) = \sum_{n=1}^3 t_0 e^{\beta(|(I+\bar{\epsilon})\mathbf{d}_n|/|\mathbf{d}_n|-1)} e^{-i\mathbf{k} \cdot [(I+\bar{\epsilon})\mathbf{d}_n]}, \quad (\text{A.2})$$

in the high-symmetry points, we have that

$$\sum_{n=1}^3 t_n e^{-i\mathbf{K}_D \cdot [(I+\bar{\epsilon})\mathbf{d}_n]} = 0 \quad (\text{A.3})$$

where $t_n = t_0 e^{\beta(|(I+\bar{\epsilon})\mathbf{d}_n|/|\mathbf{d}_n|-1)}$. Continuing, we will evaluate whether there is a difference in tensioning the real lattice or the reciprocal lattice, thus

$$\mathbf{K}_D \cdot [(I + \bar{\epsilon})\mathbf{d}_n] = k_{0x} [\epsilon_{xy} d_y^j + d_x^j (\epsilon_{xx} + 1)] + k_{0y} [\epsilon_{yx} d_x^j + d_y^j (\epsilon_{yy} + 1)] \quad (\text{A.4})$$

$$[(I + \bar{\epsilon})\mathbf{K}_D] \cdot \mathbf{d}_n = k_{0x} [\epsilon_{yx} d_y^j + d_x^j (\epsilon_{xx} + 1)] + k_{0y} [\epsilon_{xy} d_x^j + d_y^j (\epsilon_{yy} + 1)]. \quad (\text{A.5})$$

Comparing them, we note that except for the cases of deformation SX and SY, the equality holds $\mathbf{K}_D \cdot [(I + \bar{\epsilon})\mathbf{d}_n] = [(I + \bar{\epsilon})\mathbf{K}_D] \cdot \mathbf{d}_n$, in general the following relationship applies $\mathbf{K}_D \cdot [(I + \bar{\epsilon})\mathbf{d}_n] = [(I + \bar{\epsilon})^T \mathbf{K}_D] \cdot \mathbf{d}_n$, then we will define $\mathbf{G} = (I + \bar{\epsilon})^T \mathbf{K}_D$, this case

$$\sum_{n=1}^3 t_n e^{-i\mathbf{G} \cdot \mathbf{d}_n} = 0. \quad (\text{A.6})$$

Now, let's expand $\mathbf{G}$ in terms of the strain amplitude ϵ with second-order approximation around a point of high symmetry $\mathbf{K}_0$, in this way

$$\mathbf{G} = \mathbf{K}_0 + \mathbf{A}^{(1)} + \mathbf{A}^{(2)} + O(\epsilon^3). \quad (\text{A.7})$$

We know that hopping also changes with strain, so let's consider the same approximation in the same way, like this

$$t_n/t_0 = 1 + \Delta_n^{(1)} + \Delta_n^{(2)} + O(\epsilon^3). \quad (\text{A.8})$$

Let us substitute Eqs. (A.7) and (A.8) in the Eq. (A.6), thus

$$\sum_{n=1}^3 t_n e^{-i\mathbf{G} \cdot \mathbf{d}_n} \approx \sum_{n=1}^3 (1 + \Delta_n^{(1)} + \Delta_n^{(2)}) e^{-i(\mathbf{K}_0 + \mathbf{A}^{(1)} + \mathbf{A}^{(2)}) \cdot \mathbf{d}_n} = 0 \quad (\text{A.9})$$

considering only second-order corrections in the strain amplitude, we have

$$e^{-i\mathbf{A}^{(j)} \cdot \mathbf{d}_n} \approx 1 - i\mathbf{A}^{(j)} \cdot \mathbf{d}_n - \frac{(\mathbf{A}^{(j)} \cdot \mathbf{d}_n)^2}{2} \quad (\text{A.10})$$

thus, disregarding terms of order greater than $O(\epsilon^2)$

$$\begin{aligned} \sum_{n=1}^3 t_n e^{-i\mathbf{G} \cdot \mathbf{d}_n} &\approx t_0 \sum_{n=1}^3 (1 + \Delta_n^{(1)} + \Delta_n^{(2)}) e^{-i\mathbf{K}_0 \cdot \mathbf{d}_n} \prod_j \left[1 - i\mathbf{A}^{(j)} \cdot \mathbf{d}_n - \frac{(\mathbf{A}^{(j)} \cdot \mathbf{d}_n)^2}{2} \right] \\ &= t_0 \sum_{n=1}^3 (1 + \Delta_n^{(1)} + \Delta_n^{(2)}) e^{-i\mathbf{K}_0 \cdot \mathbf{d}_n} \left[1 - i\mathbf{A}^{(1)} \cdot \mathbf{d}_n - \frac{(\mathbf{A}^{(1)} \cdot \mathbf{d}_n)^2}{2} \right] \\ &\quad \times \left[1 - i\mathbf{A}^{(2)} \cdot \mathbf{d}_n - \underbrace{\frac{(\mathbf{A}^{(2)} \cdot \mathbf{d}_n)^2}{2}}_{O(\epsilon^4)} \right] \\ &\approx t_0 \sum_{n=1}^3 (1 + \Delta_n^{(1)} + \Delta_n^{(2)}) e^{-i\mathbf{K}_0 \cdot \mathbf{d}_n} \left[1 - i\mathbf{A}^{(1)} \cdot \mathbf{d}_n - \frac{(\mathbf{A}^{(1)} \cdot \mathbf{d}_n)^2}{2} \right] \left[1 - i\mathbf{A}^{(2)} \cdot \mathbf{d}_n \right] \\ &= t_0 \sum_{n=1}^3 (1 + \Delta_n^{(1)} + \Delta_n^{(2)}) e^{-i\mathbf{K}_0 \cdot \mathbf{d}_n} \left[1 - i\mathbf{A}^{(1)} \cdot \mathbf{d}_n - \frac{(\mathbf{A}^{(1)} \cdot \mathbf{d}_n)^2}{2} - \right. \\ &\quad \left. - i\mathbf{A}^{(2)} \cdot \mathbf{d}_n - \underbrace{(\mathbf{A}^{(1)} \cdot \mathbf{d}_n)(\mathbf{A}^{(2)} \cdot \mathbf{d}_n)}_{O(\epsilon^3)} + \underbrace{(i\mathbf{A}^{(2)} \cdot \mathbf{d}_n) \frac{(\mathbf{A}^{(1)} \cdot \mathbf{d}_n)^2}{2}}_{O(\epsilon^4)} \right] \\ &\approx t_0 \sum_{n=1}^3 (1 + \Delta_n^{(1)} + \Delta_n^{(2)}) e^{-i\mathbf{K}_0 \cdot \mathbf{d}_n} \left[1 - i\mathbf{A}^{(1)} \cdot \mathbf{d}_n - i\mathbf{A}^{(2)} \cdot \mathbf{d}_n - \frac{(\mathbf{A}^{(1)} \cdot \mathbf{d}_n)^2}{2} \right] \\ &= t_0 \sum_{n=1}^3 e^{-i\mathbf{K}_0 \cdot \mathbf{d}_n} \left[1 - i\mathbf{A}^{(1)} \cdot \mathbf{d}_n - i\mathbf{A}^{(2)} \cdot \mathbf{d}_n - \frac{(\mathbf{A}^{(1)} \cdot \mathbf{d}_n)^2}{2} \right] \\ &\quad + t_0 \sum_{n=1}^3 e^{-i\mathbf{K}_0 \cdot \mathbf{d}_n} \left[\Delta_n^{(1)} - i\Delta_n^{(1)} \mathbf{A}^{(1)} \cdot \mathbf{d}_n - \underbrace{i\Delta_n^{(1)} \mathbf{A}^{(2)} \cdot \mathbf{d}_n}_{O(\epsilon^3)} - \underbrace{\Delta_n^{(1)} \frac{(\mathbf{A}^{(1)} \cdot \mathbf{d}_n)^2}{2}}_{O(\epsilon^3)} \right] \\ &\quad + t_0 \sum_{n=1}^3 e^{-i\mathbf{K}_0 \cdot \mathbf{d}_n} \left[\Delta_n^{(2)} - \underbrace{i\Delta_n^{(2)} \mathbf{A}^{(1)} \cdot \mathbf{d}_n}_{O(\epsilon^3)} - \underbrace{i\Delta_n^{(2)} \mathbf{A}^{(2)} \cdot \mathbf{d}_n}_{O(\epsilon^4)} - \underbrace{\Delta_n^{(2)} \frac{(\mathbf{A}^{(1)} \cdot \mathbf{d}_n)^2}{2}}_{O(\epsilon^3)} \right] \end{aligned} \quad (\text{A.11})$$

finally, separating the terms according to the order, we have

$$\begin{aligned} \sum_{n=1}^3 t_n e^{-i\mathbf{G} \cdot \mathbf{d}_n} &\approx t_0 \sum_{n=1}^3 e^{-i\mathbf{K}_0 \cdot \mathbf{d}_n} + t_0 \sum_{n=1}^3 e^{-i\mathbf{K}_0 \cdot \mathbf{d}_n} \left[\Delta_n^{(1)} - i\mathbf{A}^{(1)} \cdot \mathbf{d}_n \right] \\ &\quad + t_0 \sum_{n=1}^3 e^{-i\mathbf{K}_0 \cdot \mathbf{d}_n} \left[\Delta_n^{(2)} - i\Delta_n^{(1)} \mathbf{A}^{(1)} \cdot \mathbf{d}_n - i\Delta_n^{(1)} \mathbf{A}^{(2)} \cdot \mathbf{d}_n - \frac{(\mathbf{A}^{(1)} \cdot \mathbf{d}_n)^2}{2} \right]. \end{aligned} \quad (\text{A.12})$$

We know that at unstressed points of high symmetry the following relation holds:

$$\sum_{n=1}^3 e^{-i\mathbf{K}_0 \cdot \mathbf{d}_n} = 0, \text{ this}$$

$$\sum_{n=1}^3 e^{-i\mathbf{K}_0 \cdot \mathbf{d}_n} \left[\Delta_n^{(1)} - i\mathbf{A}^{(1)} \cdot \mathbf{d}_n \right] = 0 \quad (\text{A.13})$$

and

$$\sum_{n=1}^3 e^{-i\mathbf{K}_0 \cdot \mathbf{d}_n} \left[\Delta_n^{(2)} - i\Delta_n^{(1)} \mathbf{A}^{(1)} \cdot \mathbf{d}_n - i\mathbf{A}^{(2)} \cdot \mathbf{d}_n - \frac{(\mathbf{A}^{(1)} \cdot \mathbf{d}_n)^2}{2} \right] = 0. \quad (\text{A.14})$$

At this point, we will evaluate the hopping term t_n , considering a second-order approximation in terms of the strain amplitude ϵ , in this way

$$t_n/t_0 = e^{-\beta \left(\frac{|\mathbf{d}'_n|}{d_n} - 1 \right)} = e^{-\beta \left\{ \frac{[(I+\bar{\epsilon})\mathbf{d}_n \cdot (I+\bar{\epsilon})\mathbf{d}_n]^{1/2}}{d_n} - 1 \right\}} = e^{-\beta \left\{ \left[1 + \frac{2\mathbf{d}_n \cdot \bar{\epsilon}\mathbf{d}_n + |\bar{\epsilon}\mathbf{d}_n|^2}{d_n^2} \right]^{1/2} - 1 \right\}} \quad (\text{A.15})$$

here we will use the binomial expansion $((1+x)^{1/2} = 1 + x/2 - x^2/8 + \dots)$ and the exponential expanding in Taylor series $(e^{-ax} = 1 - ax + (ax)^2/2! - (ax)^3/3! + \dots)$, to rewrite Eq. (A.15), so

$$\begin{aligned} t_n/t_0 &= e^{-\beta \left\{ \frac{\mathbf{d}_n \cdot \bar{\epsilon}\mathbf{d}_n}{a^2} + \frac{|\bar{\epsilon}\mathbf{d}_n|^2}{2a^2} - \frac{(\mathbf{d}_n \cdot \bar{\epsilon}\mathbf{d}_n)^2}{2a^4} + O(\epsilon^3) \right\}} \\ &\approx 1 - \frac{\beta}{a^2} \mathbf{d}_n \cdot \bar{\epsilon}\mathbf{d}_n - \frac{\beta}{2a^2} |\bar{\epsilon}\mathbf{d}_n|^2 + \frac{\beta(\beta+1)}{2a^4} (\mathbf{d}_n \cdot \bar{\epsilon}\mathbf{d}_n)^2 \end{aligned} \quad (\text{A.16})$$

Comparing Eqs. (A.7) and (A.16) we get,

$$\Delta_n^{(1)} = -\frac{\beta}{a^2} \mathbf{d}_n \cdot \bar{\epsilon}\mathbf{d}_n \quad (\text{A.17})$$

$$\Delta_n^{(2)} = -\frac{\beta}{2a^2} |\bar{\epsilon}\mathbf{d}_n|^2 + \frac{\beta(\beta+1)}{2a^4} (\mathbf{d}_n \cdot \bar{\epsilon}\mathbf{d}_n)^2. \quad (\text{A.18})$$

Let us now return to Eq. (A.13), talking $\mathbf{A}^{(1)} = (A_x^{(1)} \ A_y^{(1)})^T$, $\mathbf{K}_0 = (K_{0x} \ K_{0y})^T$ and

$$\mathbf{d}_n = (d_x^n \ d_y^n)^T$$

$$\begin{aligned} \sum_{n=1}^3 e^{-i\mathbf{K}_0 \cdot \mathbf{d}_n} \left[\Delta_n^{(1)} - i\mathbf{A}^{(1)} \cdot \mathbf{d}_n \right] &= e^{-i[K_{0x}d_x^1 + K_{0y}d_y^1]} \left[\Delta_1^{(1)} - iA_x^{(1)}d_x^1 - iA_y^{(1)}d_y^1 \right] \\ &\quad + e^{-i[K_{0x}d_x^2 + K_{0y}d_y^2]} \left[\Delta_2^{(1)} - iA_x^{(1)}d_x^2 - iA_y^{(1)}d_y^2 \right] \\ &\quad + e^{-i[K_{0x}d_x^3 + K_{0y}d_y^3]} \left[\Delta_3^{(1)} - iA_x^{(1)}d_x^3 - iA_y^{(1)}d_y^3 \right] = 0 \end{aligned} \quad (\text{A.19})$$

In our case $\mathbf{d}_1 = (0 \ 1)^T a$, $\mathbf{d}_2 = (-\sqrt{3} \ -1)^T a/2$ and $\mathbf{d}_3 = (\sqrt{3} \ -1)^T a/2$, in this way

$$\begin{aligned} e^{-iK_{0y}a} \left[\Delta_1^{(1)} - iA_y^{(1)}a \right] &+ e^{iK_{0x}a\sqrt{3}/2} e^{iK_{0y}a/2} \left[\Delta_2^{(1)} + iA_x^{(1)}a\sqrt{3}/2 + iA_y^{(1)}a/2 \right] \\ &+ e^{-iK_{0x}a\sqrt{3}/2} e^{iK_{0y}a/2} \left[\Delta_3^{(1)} - iA_x^{(1)}a\sqrt{3}/2 + iA_y^{(1)}a/2 \right] = 0 \end{aligned} \quad (\text{A.20})$$

multiplying by $e^{-iK_{0y}a/2}$ and rearranging the similar terms, we obtain

$$A_x^{(1)}a\sqrt{3}\sin(K_{0x}a\sqrt{3}/2) + iA_y^{(1)}a\left[e^{-\frac{3}{2}iK_{0y}} - \cos(K_{0x}a\sqrt{3}/2)\right] = \Delta_1^{(1)}e^{-\frac{3}{2}iK_{0y}} + \Delta_2^{(1)}e^{i\frac{\sqrt{3}}{2}aK_{0x}} + \Delta_3^{(1)}e^{-i\frac{\sqrt{3}}{2}aK_{0x}} \quad (\text{A.21})$$

here, we can separate the real and imaginary parts¹ so that we can isolate $A_x^{(1)}$ and $A_y^{(1)}$,

$$A_x^{(1)} = \frac{\csc(K_{0x}a\sqrt{3}/2)}{a\sqrt{3}} \left[\Delta_1^{(1)}\text{Re}(e^{-\frac{3}{2}iK_{0y}}) + (\Delta_2^{(1)} + \Delta_3^{(1)})\text{Re}(e^{-i\frac{\sqrt{3}}{2}aK_{0x}}) \right] \quad (\text{A.22})$$

$$A_y^{(1)} = \frac{1}{a[\text{Re}(e^{-\frac{3}{2}iK_{0y}}) - \cos(K_{0x}a\sqrt{3}/2)]} \left[(\Delta_2^{(1)} - \Delta_3^{(1)})\text{Im}(e^{i\frac{\sqrt{3}}{2}aK_{0x}}) \right]. \quad (\text{A.23})$$

Continuing, we can similarly find the second-order terms,

$$A_x^{(2)}a\sqrt{3}\sin(K_{0x}a\sqrt{3}/2) + iA_y^{(2)}a\left[e^{-\frac{3}{2}iK_{0y}} - \cos(K_{0x}a\sqrt{3}/2)\right] = e^{-iK_{0y}a/2} \sum_{n=1}^3 e^{-i\mathbf{K}_0 \cdot \mathbf{d}_n} \left[\Delta_n^{(2)} - i\Delta_n^{(1)}\mathbf{A}^{(1)} \cdot \mathbf{d}_n - \frac{(\mathbf{A}^{(1)} \cdot \mathbf{d}_n)^2}{2} \right] \quad (\text{A.24})$$

now separating the like terms, we have

$$A_x^{(2)} = \frac{\csc(K_{0x}a\sqrt{3}/2)}{a\sqrt{3}} \text{Re} \left\{ \sum_{n=1}^3 e^{-i(\mathbf{K}_0 \cdot \mathbf{d}_n + K_{0y}a/2)} \left[\Delta_n^{(2)} - i\Delta_n^{(1)}\mathbf{A}^{(1)} \cdot \mathbf{d}_n - \frac{(\mathbf{A}^{(1)} \cdot \mathbf{d}_n)^2}{2} \right] \right\} \quad (\text{A.25})$$

$$A_y^{(2)} = \frac{1}{a[e^{-\frac{3}{2}iK_{0y}} - \cos(K_{0x}a\sqrt{3}/2)]} \text{Im} \left\{ \sum_{n=1}^3 e^{-i(\mathbf{K}_0 \cdot \mathbf{d}_n + K_{0y}a/2)} \left[\Delta_n^{(2)} - i\Delta_n^{(1)}\mathbf{A}^{(1)} \cdot \mathbf{d}_n - \frac{(\mathbf{A}^{(1)} \cdot \mathbf{d}_n)^2}{2} \right] \right\} \quad (\text{A.26})$$

here we consider the following properties of complex numbers: $\text{Re}(XY) = \text{Re}(X)\text{Re}(Y) - \text{Im}(X)\text{Im}(Y)$ and $\text{Im}(XY) = \text{Re}(X)\text{Im}(Y) + \text{Im}(X)\text{Re}(Y)$, thus

$$A_x^{(2)} = \frac{\csc(K_{0x}a\sqrt{3}/2)}{a\sqrt{3}} \sum_{n=1}^3 \text{Re} \left[e^{-i(\mathbf{K}_0 \cdot \mathbf{d}_n + K_{0y}a/2)} \left[\Delta_n^{(2)} - \frac{(\mathbf{A}^{(1)} \cdot \mathbf{d}_n)^2}{2} \right] \right] + \text{Im} \left[e^{-i(\mathbf{K}_0 \cdot \mathbf{d}_n + K_{0y}a/2)} \left[\Delta_n^{(1)}\mathbf{A}^{(1)} \cdot \mathbf{d}_n \right] \right] \quad (\text{A.27})$$

¹ Here it is worth highlighting the passage from Eq. (A.21) for the Eq. (A.23), since in order to separate into real and imaginary parts it is known that the term $iA_y^{(1)}a\left[e^{-\frac{3}{2}iK_{0y}} - \cos(K_{0x}a\sqrt{3}/2)\right]$ need to be pure imaginary, and it is, since the imaginary part of $e^{-\frac{3}{2}iK_{0y}}$ will be identically zero at the points of high symmetry.

$$A_y^{(2)} = \frac{1}{a[Re(e^{-\frac{3}{2}iK_{0y}}) - \cos(K_{0x}a\sqrt{3}/2)]} \sum_{n=1}^3 -Re[e^{-i(\mathbf{K}_0 \cdot \mathbf{d}_n + K_{0y}a/2)}] \left[\Delta_n^{(1)} \mathbf{A}^{(1)} \cdot \mathbf{d}_n \right] + Im[e^{-i(\mathbf{K}_0 \cdot \mathbf{d}_n + K_{0y}a/2)}] \left[\Delta_n^{(2)} - \frac{(\mathbf{A}^{(1)} \cdot \mathbf{d}_n)^2}{2} \right]. \quad (\text{A.28})$$

With the generic first and second order terms in hand, let us try to find a particular case in which $\mathbf{K} = (4\pi/(3\sqrt{3}a), 0)$, thus, through some manipulations, we obtain the following results for the first order terms

$$A_x^{(1)} = \frac{\beta(\epsilon_{xx} - \epsilon_{yy})}{2a}, \quad (\text{A.29})$$

$$A_y^{(1)} = \frac{-\beta(\epsilon_{xy} + \epsilon_{yx})}{2a}. \quad (\text{A.30})$$

For the second-order terms, we obtain

$$A_x^{(2)} = \frac{-4\beta^2(\epsilon_{xy} + \epsilon_{yx})^2 + \beta(\epsilon_{xx} - \epsilon_{yy})^2(4\beta + 1) + \beta(-5\epsilon_{xy}^2 - 2\epsilon_{xy}\epsilon_{yx} + 3\epsilon_{yx}^2)}{16a}, \quad (\text{A.31})$$

$$A_y^{(2)} = \frac{\beta(4\epsilon_{xx}\epsilon_{xy}\beta - \epsilon_{xx}\epsilon_{xy} + 4\epsilon_{xx}\epsilon_{yx}\beta + 3\epsilon_{xx}\epsilon_{yx} - 4\epsilon_{xy}\epsilon_{yy}\beta + \epsilon_{xy}\epsilon_{yy} - 4\epsilon_{yx}\epsilon_{yy}\beta - 3\epsilon_{yx}\epsilon_{yy})}{8a}. \quad (\text{A.32})$$

Here we will consider a special case where the simple shear terms are the same in the xy directions ($\epsilon_{xy} = \epsilon_{yx}$) to compare the results obtained with the work on which we are based, thus the Eqs are reduced to

$$A_x^{(1)} = \frac{\beta(\epsilon_{xx} - \epsilon_{yy})}{2a}, \quad (\text{A.33})$$

$$A_y^{(1)} = \frac{-\beta\epsilon_{xy}}{a}, \quad (\text{A.34})$$

$$A_x^{(2)} = \frac{\beta(4\beta + 1)[(\epsilon_{xx} - \epsilon_{yy})^2 - 4\epsilon_{xy}^2]}{16a}, \quad (\text{A.35})$$

$$A_y^{(2)} = \frac{\beta(4\beta + 1)(\epsilon_{xx}\epsilon_{xy} - \epsilon_{yy}\epsilon_{xy})}{4a}. \quad (\text{A.36})$$

The results we obtained agree with those of Oliva-Leyva e Wang (2017) for first-order terms and for second-order cases. For other high-symmetry points, the values are the same, minus a global signal.

APPENDIX B – EFFECTIVE DIRAC HAMILTONIAN FOR STRAINED $\alpha - T_3$ LATTICE

The Hamiltonian of the lattice $\alpha - T_3$ under deformation effect is

$$H = \sum_{n=1}^3 t_n \begin{pmatrix} 0 & e^{-i\mathbf{k} \cdot [(I+\bar{\epsilon})\mathbf{d}_n]} & \alpha t_A e^{i\mathbf{k} \cdot [(I+\bar{\epsilon})\mathbf{d}_n]} \\ e^{i\mathbf{k} \cdot [(I+\bar{\epsilon})\mathbf{d}_n]} & 0 & \alpha t_B e^{-i\mathbf{k} \cdot [(I+\bar{\epsilon})\mathbf{d}_n]} \\ \alpha t_A e^{-i\mathbf{k} \cdot [(I+\bar{\epsilon})\mathbf{d}_n]} & \alpha t_B e^{i\mathbf{k} \cdot [(I+\bar{\epsilon})\mathbf{d}_n]} & 0 \end{pmatrix}. \quad (\text{B.1})$$

Considering an effective model, with $\mathbf{k} = \mathbf{K}_D + \mathbf{q}$, we can rewrite it as

$$H = \begin{pmatrix} 0 & h & \alpha t_A h^* \\ h^* & 0 & \alpha t_B h \\ \alpha t_A h & \alpha t_B h^* & 0 \end{pmatrix}. \quad (\text{B.2})$$

in which

$$h = \sum_{n=1}^3 t_n e^{-i(\mathbf{K}_D + \mathbf{q}) \cdot [(I+\bar{\epsilon})\mathbf{d}_n]}, \quad (\text{B.3})$$

thus

$$\begin{aligned} h &= \sum_{n=1}^3 t_n e^{-i[\mathbf{K}_D \cdot (I+\bar{\epsilon})\mathbf{d}_n + \mathbf{q} \cdot (I+\bar{\epsilon})\mathbf{d}_n]} \approx \sum_{n=1}^3 t_n e^{-i[(\mathbf{K}_0 + \mathbf{A}^{(1)} + \mathbf{A}^{(2)}) \cdot (I+\bar{\epsilon})\mathbf{d}_n + \mathbf{q} \cdot (I+\bar{\epsilon})\mathbf{d}_n]} \\ &= \sum_{n=1}^3 t_n e^{-i(\mathbf{K}_0 \cdot \mathbf{d}_n)} e^{-i(\mathbf{A}^{(1)} + \mathbf{A}^{(2)}) \cdot \mathbf{d}_n} e^{-i(\mathbf{q} \cdot (I+\bar{\epsilon})\mathbf{d}_n)} \\ &= - \sum_{n=1}^3 t_n e^{-i(\mathbf{K}_0 \cdot \mathbf{d}_n)} \left[1 + i\mathbf{A}^{(1)} \cdot \mathbf{d}_n + i\mathbf{A}^{(2)} \cdot \mathbf{d}_n - \frac{(\mathbf{A}^{(1)} \cdot \mathbf{d}_n)^2}{2} \right] [1 + i\mathbf{q} \cdot (I+\bar{\epsilon})\mathbf{d}_n] \\ &= - \sum_{n=1}^3 t_n e^{-i(\mathbf{K}_0 \cdot \mathbf{d}_n)} \left[1 + i\mathbf{A}^{(1)} \cdot \mathbf{d}_n + i\mathbf{A}^{(2)} \cdot \mathbf{d}_n - \frac{(\mathbf{A}^{(1)} \cdot \mathbf{d}_n)^2}{2} + i\mathbf{q} \cdot (I+\bar{\epsilon})\mathbf{d}_n - \right. \\ &\quad \left. - (\mathbf{A}^{(1)} \cdot \mathbf{d}_n)(\mathbf{q} \cdot (I+\bar{\epsilon})\mathbf{d}_n) - (\mathbf{A}^{(2)} \cdot \mathbf{d}_n)(\mathbf{q} \cdot (I+\bar{\epsilon})\mathbf{d}_n) - i(\mathbf{A}^{(1)} \cdot \mathbf{d}_n)^2(\mathbf{q} \cdot (I+\bar{\epsilon})\mathbf{d}_n)/2 \right], \end{aligned} \quad (\text{B.4})$$

now substituting the approximating hopping term, we have

$$\begin{aligned} h &\approx -t_0 \sum_{n=1}^3 e^{-i(\mathbf{K}_0 \cdot \mathbf{d}_n)} \left[1 + \Delta_n^{(1)} + \Delta_n^{(2)} \right] \left[1 + i\mathbf{A}^{(1)} \cdot \mathbf{d}_n + i\mathbf{A}^{(2)} \cdot \mathbf{d}_n - \frac{(\mathbf{A}^{(1)} \cdot \mathbf{d}_n)^2}{2} \right. \\ &\quad \left. + i\mathbf{q} \cdot \mathbf{d}_n + \mathbf{q} \cdot \bar{\epsilon}\mathbf{d}_n - (\mathbf{A}^{(1)} \cdot \mathbf{d}_n)(\mathbf{q} \cdot \mathbf{d}_n) - (\mathbf{A}^{(1)} \cdot \mathbf{d}_n)(\mathbf{q} \cdot \bar{\epsilon}\mathbf{d}_n) \right. \\ &\quad \left. - (\mathbf{A}^{(2)} \cdot \mathbf{d}_n)(\mathbf{q} \cdot \mathbf{d}_n) - i(\mathbf{A}^{(1)} \cdot \mathbf{d}_n)^2(\mathbf{q} \cdot \mathbf{d}_n)/2 \right], \end{aligned} \quad (\text{B.5})$$

distributing the terms

$$\begin{aligned}
h \approx & -t_0 \sum_{n=1}^3 e^{-i(\mathbf{K}_0 \cdot \mathbf{d}_n)} \left[1 + i\mathbf{A}^{(1)} \cdot \mathbf{d}_n + i\mathbf{A}^{(2)} \cdot \mathbf{d}_n - \frac{(\mathbf{A}^{(1)} \cdot \mathbf{d}_n)^2}{2} + i\mathbf{q} \cdot \mathbf{d}_n + \mathbf{q} \cdot \bar{\epsilon} \mathbf{d}_n \right. \\
& - (\mathbf{A}^{(1)} \cdot \mathbf{d}_n)(\mathbf{q} \cdot \mathbf{d}_n) - (\mathbf{A}^{(1)} \cdot \mathbf{d}_n)(\mathbf{q} \cdot \bar{\epsilon} \mathbf{d}_n) - (\mathbf{A}^{(2)} \cdot \mathbf{d}_n)(\mathbf{q} \cdot \mathbf{d}_n) - i \frac{(\mathbf{A}^{(1)} \cdot \mathbf{d}_n)^2}{2} (\mathbf{q} \cdot \mathbf{d}_n) \\
& + \Delta_n^{(1)} + i\Delta_n^{(1)} \mathbf{A}^{(1)} \cdot \mathbf{d}_n + i\Delta_n^{(1)} \mathbf{A}^{(2)} \cdot \mathbf{d}_n - \Delta_n^{(1)} \frac{(\mathbf{A}^{(1)} \cdot \mathbf{d}_n)^2}{2} + i\Delta_n^{(1)} \mathbf{q} \cdot \mathbf{d}_n + \Delta_n^{(1)} \mathbf{q} \cdot \bar{\epsilon} \mathbf{d}_n \\
& - \Delta_n^{(1)} (\mathbf{A}^{(1)} \cdot \mathbf{d}_n)(\mathbf{q} \cdot \mathbf{d}_n) - \Delta_n^{(1)} (\mathbf{A}^{(1)} \cdot \mathbf{d}_n)(\mathbf{q} \cdot \bar{\epsilon} \mathbf{d}_n) - \Delta_n^{(1)} (\mathbf{A}^{(2)} \cdot \mathbf{d}_n)(\mathbf{q} \cdot \mathbf{d}_n) \\
& - i\Delta_n^{(1)} \frac{(\mathbf{A}^{(1)} \cdot \mathbf{d}_n)^2}{2} (\mathbf{q} \cdot \mathbf{d}_n) + \Delta_n^{(2)} + i\Delta_n^{(2)} \mathbf{A}^{(1)} \cdot \mathbf{d}_n + i\Delta_n^{(2)} \mathbf{A}^{(2)} \cdot \mathbf{d}_n - \Delta_n^{(2)} \frac{(\mathbf{A}^{(1)} \cdot \mathbf{d}_n)^2}{2} \\
& + i\Delta_n^{(1)} \mathbf{q} \cdot \mathbf{d}_n + \Delta_n^{(2)} \mathbf{q} \cdot \bar{\epsilon} \mathbf{d}_n - \Delta_n^{(2)} (\mathbf{A}^{(1)} \cdot \mathbf{d}_n)(\mathbf{q} \cdot \mathbf{d}_n) - \Delta_n^{(2)} (\mathbf{A}^{(1)} \cdot \mathbf{d}_n)(\mathbf{q} \cdot \bar{\epsilon} \mathbf{d}_n) \\
& \left. - \Delta_n^{(2)} (\mathbf{A}^{(2)} \cdot \mathbf{d}_n)(\mathbf{q} \cdot \mathbf{d}_n) - i\Delta_n^{(2)} \frac{(\mathbf{A}^{(1)} \cdot \mathbf{d}_n)^2}{2} (\mathbf{q} \cdot \mathbf{d}_n) \right],
\end{aligned}$$

discarding terms of order $O(\epsilon^3)$, we have

$$\begin{aligned}
h \approx & -t_0 \sum_{n=1}^3 e^{-i(\mathbf{K}_0 \cdot \mathbf{d}_n)} \left[\underbrace{1 + i\mathbf{A}^{(1)} \cdot \mathbf{d}_n + i\mathbf{A}^{(2)} \cdot \mathbf{d}_n - \frac{(\mathbf{A}^{(1)} \cdot \mathbf{d}_n)^2}{2} + \Delta_n^{(1)} + i\Delta_n^{(1)} \mathbf{A}^{(1)} \cdot \mathbf{d}_n + \Delta_n^{(2)}}_{=0} \right. \\
& + \underbrace{i\mathbf{q} \cdot \mathbf{d}_n}_{h_0} + \underbrace{i\mathbf{q} \cdot \bar{\epsilon} \mathbf{d}_n}_{h_{1,a}} - \underbrace{(\mathbf{A}^{(1)} \cdot \mathbf{d}_n)(\mathbf{q} \cdot \mathbf{d}_n) + i\Delta_n^{(1)}(\mathbf{q} \cdot \mathbf{d}_n)}_{h_{1,b}} - \underbrace{(\mathbf{A}^{(1)} \cdot \mathbf{d}_n)(\mathbf{q} \cdot \bar{\epsilon} \mathbf{d}_n) + i\Delta_n^{(1)}(\mathbf{q} \cdot \bar{\epsilon} \mathbf{d}_n)}_{h_{2,a}} \\
& \left. - \underbrace{i \frac{(\mathbf{A}^{(1)} \cdot \mathbf{d}_n)^2}{2} (\mathbf{q} \cdot \mathbf{d}_n) - \Delta_n^{(1)} (\mathbf{A}^{(1)} \cdot \mathbf{d}_n)(\mathbf{q} \cdot \mathbf{d}_n) - (\mathbf{A}^{(2)} \cdot \mathbf{d}_n)(\mathbf{q} \cdot \mathbf{d}_n) + i\Delta_n^{(2)} (\mathbf{q} \cdot \mathbf{d}_n)}_{h_{2,b}} \right],
\end{aligned}$$

finally, we can rewrite the structure factor with a second-order approximation in strain as

$$h \approx h_0 + h_{1,a} + h_{1,b} + h_{2,a} + h_{2,b} \quad (\text{B.6})$$

in which

$$h_0 = -t_0 \sum_{n=1}^3 e^{-i(\mathbf{K}_0 \cdot \mathbf{d}_n)} [i\mathbf{q} \cdot \mathbf{d}_n] \quad (\text{B.7})$$

$$h_{1,a} = -t_0 \sum_{n=1}^3 e^{-i(\mathbf{K}_0 \cdot \mathbf{d}_n)} [i\mathbf{q} \cdot \bar{\epsilon} \mathbf{d}_n], \quad (\text{B.8})$$

$$h_{1,b} = -t_0 \sum_{n=1}^3 e^{-i(\mathbf{K}_0 \cdot \mathbf{d}_n)} [(\mathbf{A}^{(1)} \cdot \mathbf{d}_n)(\mathbf{q} \cdot \mathbf{d}_n) + i\Delta_n^{(1)} \mathbf{A}^{(1)} \cdot \mathbf{d}_n], \quad (\text{B.9})$$

$$h_{2,a} = t_0 \sum_{n=1}^3 e^{-i(\mathbf{K}_0 \cdot \mathbf{d}_n)} [-(\mathbf{A}^{(1)} \cdot \mathbf{d}_n)(\mathbf{q} \cdot \bar{\epsilon} \mathbf{d}_n) + i\Delta_n^{(1)} (\mathbf{q} \cdot \bar{\epsilon} \mathbf{d}_n)], \quad (\text{B.10})$$

$$\begin{aligned}
h_{2,b} = -t_0 \sum_{n=1}^3 e^{-i(\mathbf{K}_0 \cdot \mathbf{d}_n)} & \left[i \frac{(\mathbf{A}^{(1)} \cdot \mathbf{d}_n)^2}{2} (\mathbf{q} \cdot \mathbf{d}_n) - \Delta_n^{(1)} (\mathbf{A}^{(1)} \cdot \mathbf{d}_n) (\mathbf{q} \cdot \mathbf{d}_n) \right. \\
& \left. - (\mathbf{A}^{(2)} \cdot \mathbf{d}_n) (\mathbf{q} \cdot \mathbf{d}_n) + i \Delta_n^{(2)} (\mathbf{q} \cdot \mathbf{d}_n) \right]. \tag{B.11}
\end{aligned}$$

This derivation of the effective Hamiltonian under strain for the $\alpha - T_3$ lattice is based on the paper by Oliva-Leyva e Wang (2017) for graphene.