

This item is the archived peer-reviewed author-version of:

Band-gap formation and morphing in alpha-T-3 superlattices

Reference:

Cunha Sofia M., de Costa D.R., Pereira Jr J. Milton, Costa Filho R.N., Van Duppen Ben, Peeters François.- Band-gap formation and morphing in alpha-T-3 superlattices
Physical review B / American Physical Society - ISSN 2469-9969 - 104:11(2021), 115409
Full text (Publisher's DOI): <https://doi.org/10.1103/PHYSREVB.104.115409>
To cite this reference: <https://hdl.handle.net/10067/1815440151162165141>

Band gap formation and morphing in $\alpha - T_3$ superlattices

S. M. Cunha,^{1,2,*} D. R. da Costa,² J. Milton Pereira Jr.,² R. N. Costa Filho,² B. Van Duppen,^{1,†} and F. M. Peeters¹

¹*Department of Physics, University of Antwerp, Groenenborgerlaan 171, B-2020 Antwerp, Belgium*

²*Departamento de Física, Universidade Federal do Ceará, Campus do Pici, Fortaleza, Ceará, Brazil*

(Dated: October 6, 2021)

Electrons in $\alpha - T_3$ lattices behave as condensed-matter analogies of integer-spin Dirac Fermions. The three atoms making up the unit cell bestow the energy spectrum with an additional energy band that is completely flat, providing unique electronic properties. The interatomic hopping term, α , is known to strongly affect the electronic spectrum of the 2D lattice, allowing it to continuously morph from graphene-like responses to the behaviour of Fermions in a Dice lattice. For pristine lattice structures, the energy bands are gapless, however small deviations in the atomic equivalence of the three sublattices will introduce gaps in the spectrum. It is unknown how these affect transport and electronic properties such as the energy spectrum of superlattice mini-bands. Here we investigate the dependency of these properties on the parameter α accounting for different symmetry-breaking terms and show how it affects band gap formation. Furthermore, we find that superlattices can force band gaps to close and shift in energy. Our results demonstrate that $\alpha - T_3$ superlattices provide a versatile material for 2D band gap engineering purposes.

PACS numbers:

I. INTRODUCTION

The isolation of a stable single layer of carbon atoms arranged in a hexagonal lattice, known as graphene, in 2004¹ combined with the extraordinary electronic and transport properties observed in the atomically thin material¹⁻⁴ has motivated many researchers to investigate and produce other two-dimensional (2D) materials^{1,5-7}. The peculiar electronic properties of graphene are the result of charge carriers described by an equation analogous to the Dirac one for relativistic particles but here the presence of a variable similar to a spinor representation, differently from the "real" one, results only from the crystal structure instead from an intrinsic property of the particles. Therefore the charge carriers in graphene are commonly referenced as pseudospin-1/2 particles^{8,9}. These particles have a linear energy dispersion where valence and conduction bands touch each other in special points in reciprocal space called Dirac points^{2,3,8,9}.

2D materials can be subjected to electrostatic potentials with a periodicity significantly larger than the interatomic distance¹⁰⁻¹³. Because one can easily change the strength of the electrostatic potential, this method has been thoroughly investigated as a way to tune electronic properties of the charge carriers in these 2D systems¹⁴⁻²⁰. Superlattice potentials are known to increase the number of Dirac points of graphene^{16-18,21-24,26} and as such introduce new physical modes at zero energy, as recently observed in Ref. [25]. Some relevant applications originated from the periodic structures are electron beam supercollimation and electron wave filter^{24,26}.

Recently, novel and distinctive physics has emerged from 2D systems when adding an additional atom in their crystal structure²⁷⁻³⁴, which leads to their charge carriers in a low-energy approach to be described as enlarged pseudospin Dirac Fermions^{31,32,35-37}. Among these systems we have Lieb lattice with the additional atom at

edges of a square-lattice, which was recently obtained by adding carbon monoxide molecules to a substrate²⁸ and the T_3 or dice lattice which has an additional atom at the center of the hexagonal structure. In both, different from graphene, the massless Dirac Fermions are described as spin-1 particles and an additional flat-band touching the top of the valence and the bottom of the conduction linear bands^{38,39}. This flat band has important and unusual effects on the electronic properties due to its dispersionless nature and thus an infinity effective mass^{37-44,46}. Moreover, flat bands are predicted to be important in the search for room-temperature superconductivity^{47,48}.

The graphene hexagonal lattice and T_3 or dice lattice are incorporated in the $\alpha - T_3$ model^{38,42-46}. It allows a tuning between the central atom arrangement and the hexagonal structure by varying the parameter α . Graphene and T_3 are the limiting cases $\alpha = 0$ and $\alpha = 1$, respectively.

The $\alpha - T_3$ model has been useful to investigate physical systems presenting Dirac Fermions with a larger pseudo-spin value. The $\alpha - T_3$ model was originally proposed to describe the dia- to paramagnetic transition in the orbital susceptibility in an optical lattice of cold atoms^{49,50}. The limiting case $\alpha = 1$ corresponds to the dice lattice which can be obtained by stacking three layers of SrTiO₃/SrIrO₃/SrTiO₃⁵¹, or be generated by controlling three laser beams propagating in towards a two-dimensional layer of cold atoms⁵². Likewise this model with appropriate doping and for the case $\alpha = 1/\sqrt{3}$ can be used to describe the three-dimensional Hg_{1-x}Cd_xTe system^{53,54}.

Curiously, systems with charge carriers described as spin-1 massless Dirac Fermions, for certain energy conditions have an angular independent Klein tunneling through rectangular electrostatic barriers which is called super-Klein tunneling (SKT). This isotropic transmission

is unlike single and bilayer graphene that show highly anisotropic transmission across such barriers. In addition, the tunneling into the flat band across a potential step for generalized pseudospin has been discussed as well^{31,36}. Previous studies considering Dirac Fermions across electrostatic potentials in systems with intermediate values of α reveal perfect transmission for normal incidence, and a general trend of enhanced transmission with increasing α ^{36,45,46}. Moreover, when more barriers are considered, in the case of the dice lattice the tunneling shows little dependence on the number of barriers, whereas for graphene the number of barriers strongly affects the tunneling⁶³.

Several studies have been published aiming at a way to create a band gap in these structures^{44,55,56,60–62}. This is necessary for practical electronic applications such as the fabrication of quantum information devices. It was demonstrated that an additional mass term in $\alpha - T_3$ systems distorts the linear bands around the Dirac cone and produces an energy gap with a third band in it which could be flat or dispersive^{43,44}. The position of this band inside the band gap has important consequences for Klein tunneling of massive Dirac Fermions across potential barriers.

Motivated by the richness of the tunneling properties and the peculiar electronic properties of Dirac Fermions with integer pseudospin, and aiming at understanding how the band gap in $\alpha - T_3$ systems varies as function of the tuning parameter α in the presence of super periodicity, we investigate the energy spectra and density of states (DOS) first in ungapped $\alpha - T_3$ superlattices, and subsequently we take into account the effect of different symmetry-breaking terms. In both cases we pay special attention to the appearance of mini-bands, its band flatness, and its dependence on the coupling parameter α .

This paper is organized as follows. In the second section we discuss the electronic properties of charge carriers in $\alpha - T_3$ lattices and how this is affected by small deviations in the atomic equivalence between the sites and the presence of mass terms. In the third section we develop the transfer matrix approach to analyze the energy spectra of Dirac Fermions in $\alpha - T_3$ in the presence of a one-dimensional (1D) periodic potential. In the fourth section we discuss the band gap morphing and its dependence on (i) the coupling parameter, and (ii) the symmetry-breaking between the atomic sites by the inclusion of different mass terms. Conclusions are presented in the fifth section.

II. FERMIONS IN $\alpha - T_3$ LATTICES

A. Energy spectrum and eigenstates

An $\alpha - T_3$ lattice is formed by the superposition of three triangular sublattices³². Two of them are formed by atom sites A and B arranged in a hexagonal lattice with hopping term t . The additional site C is connected

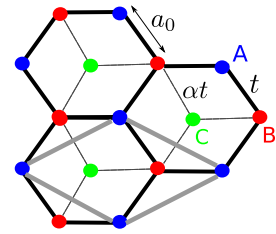


FIG. 1: Schematic of the $\alpha - T_3$ lattice where the sites of the three sublattices are coloured differently. The limit $\alpha = 0$ corresponds to the honeycomb lattice (graphene-like), and $\alpha = 1$ corresponds to the dice lattice. The hopping amplitude between the different atoms is indicated. The region bounded by the grey lines corresponds to the unit cell.

only to sites B by a hopping term tuned by a parameter α , which is the parameter that provides a continuous transition from the honeycomb ($\alpha = 0$) to the dice ($\alpha = 1$) lattice and determines the strength of coupling between the C atoms at the center of the honeycomb lattice, as shown in Fig. 1. The distance between the A , B and C atoms are the same and denoted by a_0 . The hopping parameters t , α and a_0 depend on the specific atomic composition of the lattice under consideration and completely determine the properties of the $\alpha - T_3$ lattice.

The presence of the additional site C centered in the honeycomb lattice results in some interesting electronic properties, like e.g. the presence of a flat band in addition to the linear bands and the larger value of pseudospin of charge carriers in these lattices^{31,32,38,42,46,51–54}.

The lattice structure determines the kinetic energy of the Fermions in the material. The low-energy Hamiltonian of Fermions in a $\alpha - T_3$ lattice around the K point is given by the 3×3 matrix expressed in the sublattice basis $|\Psi\rangle = (|\psi_A\rangle, |\psi_B\rangle, |\psi_C\rangle)$ as^{32,42}

$$\hat{H}_{\text{kin}} = \begin{pmatrix} 0 & f_{\xi}(\vec{k}) \cos \theta & 0 \\ f_{\xi}^*(\vec{k}) \cos \theta & 0 & f_{\xi}(\vec{k}) \sin \theta \\ 0 & f_{\xi}^*(\vec{k}) \sin \theta & 0 \end{pmatrix}. \quad (1)$$

In Eq. (1) we introduced the parameter $\theta = \tan^{-1} \alpha$, where $\theta = 0$ and $\theta = \pi/4$ corresponds to honeycomb and dice lattices, respectively. The function $f_{\xi}(\vec{k}) = v_F(\xi k_x - i k_y)$ with $v_F = 3a_0 t / 2\hbar$ the Fermi velocity and $\vec{k} = (k_x, k_y)$ the wave vector. Here, $\xi = \pm 1$ is the valley index for the K and K' valleys, respectively^{32,42}. In the absence of external potentials, the eigenstates of the Hamiltonian are given by

$$|\Psi_{\pm}\rangle = \begin{pmatrix} \cos \theta e^{i\phi_k} \\ \pm 1 \\ \sin \theta e^{-i\phi_k} \end{pmatrix}, \quad (2)$$

with eigenvalues $E_{\pm} = \pm \hbar v_F k$, where \pm indicates the conduction and valence bands, respectively. The angle $\phi_k = \tan^{-1}(k_y/k_x)$ corresponds to the angle associated with the momentum vector. In addition, a flat band state

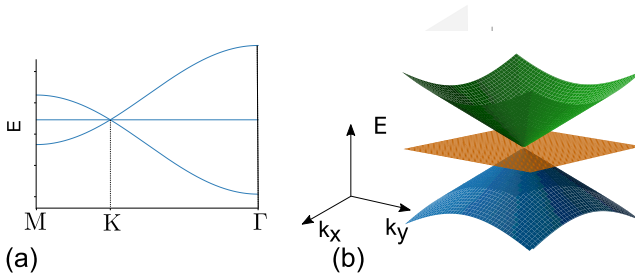


FIG. 2: Energy spectrum of massless Dirac fermions in the $\alpha - T_3$ lattice (a) in the full first Brillouin zone, and (b) around the K point.

is found

$$|\Psi_0\rangle = \begin{pmatrix} \cos \theta e^{i\phi_k} \\ 0 \\ \sin \theta e^{-i\phi_k} \end{pmatrix}, \quad (3)$$

with eigenvalue $E = 0$ corresponding to strongly degenerate states^{31,51,52}, as represented in Fig. 2. Notice that the energy eigenvalues E do not depend on θ . The parameter is solely affecting the eigenstates.

B. Introduction of a band gap

The Dirac point at $E = 0$ in the pristine $\alpha - T_3$ lattice is triple degenerate as seen in Fig. 2. This degeneracy is produced by the equivalence of the three sub-lattices. Breaking this equivalence will lead to a lifting of the degeneracy and the introduction of a band gap. In general, one can include this in the Hamiltonian by a term proportional to \hat{U} that enters as follows:

$$\hat{H} = \hat{H}_{\text{kin}} + \Delta \hat{U}, \quad (4)$$

with \hat{H}_{kin} given by Eq. (1), and Δ measures the strength of the symmetry breaking. The Hamiltonian in Eq. (4) is obtained from an expansion of the tight-binding model to nearest neighbors of the $\alpha - T_3$ lattices around the K point of the first Brillouin zone when different on-site energies are considered^{38,42,52}. In this work, we consider two different forms of \hat{U} , respectively, given by

$$\hat{U}_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \hat{U}_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \quad (5)$$

The effects of the inclusion of the terms \hat{U}_1 and \hat{U}_2 on the energy spectrum are shown in Fig. 3 and Fig. 4, respectively.

The term \hat{U}_1 introduces a site energy on the different sub-lattices as has been discussed for photonic crystals and optical lattices^{55,56}. The solution of $\hat{H}\Psi = E\Psi$ for this case gives the eigenenergies

$$E_0 = \Delta, \quad E = \pm \sqrt{\Delta^2 + \hbar^2 v_F^2 k^2}. \quad (6)$$

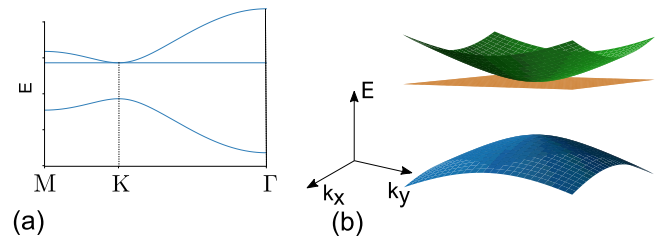


FIG. 3: Energy spectrum of Dirac Fermions for arbitrary values of the parameter θ in the $\alpha - T_3$ lattice when the symmetry-breaking term $\hat{U} = \hat{U}_1$ is used in Eq. (4). (a) Full first Brillouin zone, and (b) spectrum around the K point.

Correspondingly, the wave-functions in this case are given by

$$|\psi_0\rangle = \begin{pmatrix} \cos \theta e^{i\phi_k} \\ 0 \\ \sin \theta e^{-i\phi_k} \end{pmatrix}, \quad |\psi_{\pm}\rangle = \begin{pmatrix} \alpha \cos \theta e^{-i\phi_k} \\ \gamma \\ \alpha \sin \theta e^{i\phi_k} \end{pmatrix}, \quad (7)$$

where $\alpha = \sqrt{E + \Delta}$, and $\gamma = \sqrt{E - \Delta}$.

Similar sublattice symmetry breaking systems have been discussed suggesting that such mass potential term is attainable by depositing graphene on specific substrates, such as SiC^{57,58}, and h-BN⁵⁹. In Eq. (6) we find the presence of a gap 2Δ opening in the energy spectrum. This results in massive Dirac Fermions with an effective mass defined as $m = \Delta/v_F^2$. Since Eq. (6) does not depend on the parameter θ the energy spectrum remains the same for all $\alpha - T_3$ lattices, as shown in Fig. 3. Moreover, as long as the equivalence between the sites A and C is maintained, the flatband is shifted and touches only the bottom of the conduction band. Notice that now the bottom of the conduction band and the top of the valence band are quadratic in \vec{k} .

On the other hand, the term \hat{U}_2 defined in Eq. (5) has been used to describe the effect of a pseudomagnetic field^{60,61}, and the dispersion relations for this case are obtained from a solution of the non-linear equation

$$E(\Delta^2 - E^2) + k^2(\Delta \cos 2\theta + E) = 0, \quad (8)$$

and the eigenstate for the conduction and valence band are given by

$$|\psi\rangle = \begin{pmatrix} \alpha' \cos \theta e^{i\phi_k} \\ \gamma' \\ \beta \sin \theta e^{-i\phi_k} \end{pmatrix}, \quad (9)$$

with $\alpha' = \sqrt{1 + 2\Delta/(E - \Delta)}$, $\gamma' = \sqrt{1 + \Delta \cos(2\theta)/E}$ and $\beta = \sqrt{1 - 2\Delta/(E + \Delta)}$.

Unlike the previous case, there is no longer equivalence between the site C and the other sites of the crystal structure, which means that small deviations of the coupling parameter α results in different eigenenergies as depicted in Fig. 4. In this case the flat band is dispersionless only when $\theta = \pi/4$ (dice lattice) and is located in the center of the energy gap^{61,62}, as shown in Fig. 4(a).

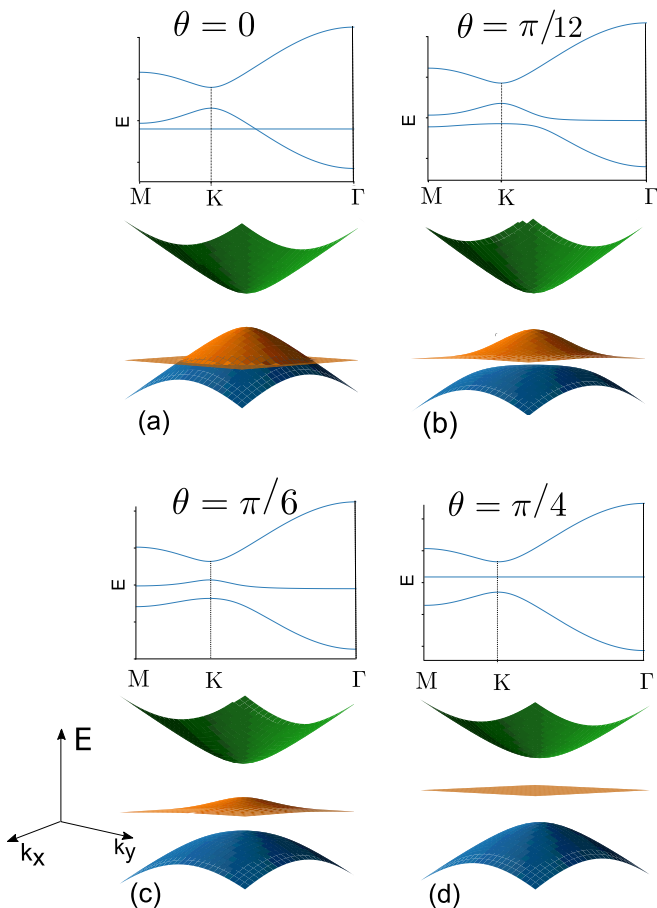


FIG. 4: Energy spectrum of Dirac Fermions in the $\alpha - T_3$ lattice for different values of θ when the symmetry-breaking term $\hat{U} = \hat{U}_2$ is used in Eq. (4). The full first Brillouin zone is shown at the top and below the energy spectrum around the K point for (a) $\theta = 0$ (graphene-like case), (b) $\theta = \pi/12$, (c) $\theta = \pi/6$, and (d) $\theta = \pi/4$ (dice case).

III. SUPERLATTICE

In this paper we investigate how fermions in $\alpha - T_3$ lattices are affected by a one-dimensional periodic electrostatic potential. In casu, we investigate one-dimensional potentials with a periodicity much larger than the interatomic distance, i.e. $L/a_0 \ll 1$. We consider an infinite number of barriers periodically spaced with unit cell length $L = W_w + W_b$, with W_w (W_b) the width of well (barrier), as illustrated in Fig. 5. The general Hamiltonian taking into account the presence of symmetry-breaking terms is now given by^{36,42,46}

$$\hat{H} = \hat{H}_{\text{kin}} + V(x)\hat{I} + \Delta\hat{U}_i, \quad (10)$$

with \hat{H}_{kin} given by Eq. (1), $V(x) = V_b$ the periodic potential, and $\Delta\hat{U}_i$ represent the symmetry-breaking term which can be translated into a mass term. Due to translation invariance in the y direction the wave-functions have the form $\Psi_j(x, y) = \Psi_j(x)e^{ik_y y}$ with label $j = w$

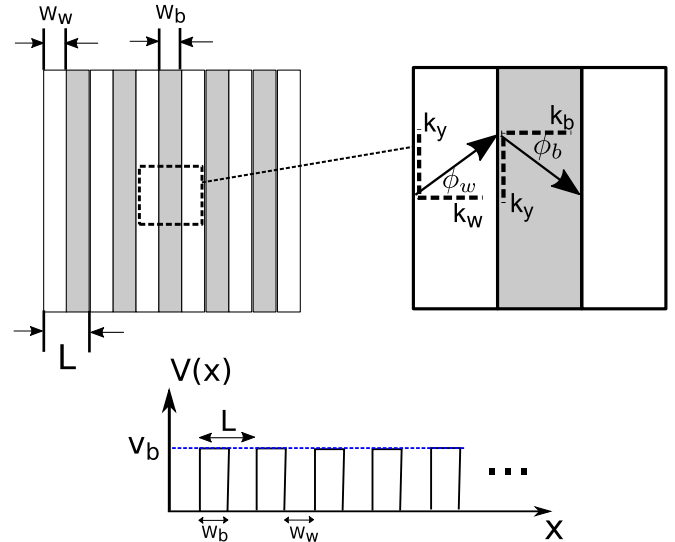


FIG. 5: Schematic representation of the superlattice potential in $x - y$ plane. Dark regions denote the barrier region with height $V(x) = V_b$ and the white region represents the well with zero potential. The angles ϕ_w and ϕ_b in the inset, respectively, denote the angles of the carriers in the wells and barriers regions. The profiles of the 1D periodic potential is given by the figure at the bottom.

or $j = b$ used to denote the region of well (barrier), and $\Psi_j(x)$ is given by:

$$\begin{aligned} \psi_j(x) = & \frac{A}{\sqrt{2}} \begin{pmatrix} \alpha_j \cos \theta e^{i\phi_j} \\ \gamma_j \\ \beta_j \sin \theta e^{-i\phi_j} \end{pmatrix} e^{ik_j x} + \\ & \frac{B}{\sqrt{2}} \begin{pmatrix} -\alpha_j \cos \theta e^{-i\phi_j} \\ \gamma_j \\ -\beta_j \sin \theta e^{i\phi_j} \end{pmatrix} e^{-ik_j x}. \end{aligned} \quad (11)$$

The angles $\phi_w = \tan^{-1}(k_y/k_w)$ and $\phi_b = \tan^{-1}(k_y/k_b)$ are the angles associated with the direction of the momentum of the electron in the well and barrier regions, respectively, as depicted in the inset of Fig. 5, and both in addition to the terms α_j , γ_j , and β_j are obtained from the eigenstates equation using the Hamiltonian Eq. (10).

Moreover, the constants A, B, C, D are determined by requesting continuity of the wave-functions. Writing the wave-functions given by Eq. (11) in the general form $\Psi(x) = (\psi_A(x), \psi_B(x), \psi_C(x))$ and by integrating the eigenvalue equation $\hat{H}\Psi = E\Psi$ over a small interval $x = [-\epsilon, \epsilon]$ and allowing the interval to approach zero, we obtain the following matching conditions for the wave-function on either side of the superlattice

$$\psi_B(-\epsilon) = \psi_B(\epsilon), \quad (12a)$$

and

$$\cos \theta \psi_A(-\epsilon) + \sin \theta \psi_C(-\epsilon) = \cos \theta \psi_A(\epsilon) + \sin \theta \psi_C(\epsilon). \quad (12b)$$

These matching conditions are different from those of the two limiting cases in the $\alpha - T_3$ model, i.e. graphene-like ($\alpha = 0$) and dice lattice ($\alpha = \pi/4$)^{13,46}. Whereas for graphene which has pseudospin-1/2 the matching conditions simply require the continuity of each two-component of the wave-function, however for the dice lattice which has integer pseudospin, the matching condition takes into account a sum of the first and last component of the three-components of the wave-function, as indicated in Eq. (12) by setting $\cos\theta = \sin\theta = 1/\sqrt{2}$. Applying the matching conditions given by Eq. (12) into Eq. (11) we obtain the transfer matrix for the $\alpha - T_3$ superlattice

$$T = \Omega_{k_w}(L)\Omega_{k_w}^{-1}(W_b)\Omega_{k_b}(W_b)\Omega_{k_b}^{-1}(0), \quad (13)$$

where

$$\Omega_{k_j}(x) = \begin{pmatrix} \gamma_j e^{ik_j x} & \gamma_j e^{-ik_j x} \\ \lambda_j e^{ik_w x} & -\lambda_j^* e^{-ik_w x} \end{pmatrix}, \quad (14)$$

with

$$\lambda_j = \cos^2\theta e^{i\phi_j} + \sin^2\theta e^{-i\phi_j}. \quad (15)$$

Inserting Eq. (14) into Eq. (13) we get:

$$T = \frac{1}{a_b a_w} \begin{pmatrix} c_+ \lambda_b^\dagger + c_- \lambda_b & \gamma_b (c_+ - c_-) \\ d_+ \lambda_b^\dagger + d_- \lambda_b & \gamma_b (d_+ - d_-) \end{pmatrix}, \quad (16)$$

where

$$a_j = \gamma_j (\lambda_j^* + \lambda_j), \quad (17a)$$

$$\begin{aligned} c_+ &= e^{ik_b W_b} \gamma_w (\gamma_b b_1 + \lambda_b b_2), \\ c_- &= e^{-ik_b W_b} \gamma_w (\gamma_b b_1 - \lambda_b^* b_2), \end{aligned} \quad (17b)$$

$$\begin{aligned} d_+ &= e^{ik_b W_b} (\gamma_b \lambda_w \lambda_w^* b_2 + \gamma_w \lambda_b b_3), \\ d_- &= e^{-ik_b W_b} (\gamma_b \lambda_w \lambda_w^* b_2 - \gamma_w \lambda_b^* b_3) \end{aligned} \quad (17c)$$

with $b_1 = \lambda_w^* e^{ik_w W_w} + \lambda_w e^{-ik_w W_w}$, $b_2 = e^{ik_w W_w} - e^{-ik_w W_w}$ and $b_3 = \lambda_w e^{ik_w W_w} + \lambda_w^* e^{-ik_w W_w}$.

According to Bloch's theorem and requiring $\det[T] = 1$ the electronic dispersion at any incident angle is given by $2\cos(K_x L) = \text{Tr}(T)$, where $K_x = 2\pi n/L$ expresses

the periodicity of the superlattice structure. This results into the following nonlinear equation for the dispersion relation

$$\begin{aligned} \cos(K_x L) &= \cos(k_b W_b) \cos(k_w W_w) \\ &\quad - G_U \sin(k_b W_b) \sin(k_w W_w), \end{aligned} \quad (18)$$

where G_U differs by the presence or absence of the symmetry-breaking term. It is denoted by G_0 for the gapless case, G_1 , and G_2 when \hat{U}_1 , and \hat{U}_2 are taken into account, respectively. As we will demonstrate further on, since the dispersion relation given in Eq. (18) depends on the symmetry between the atomic sites of the crystal structure, the inclusion of small deviations between them lead to large changes in the energy spectra and the band gap.

The allowed states for the superlattice is obtained when $-1 \leq \cos(K_x L) \leq 1$ in Eq. (18) which corresponds to the energy spectra for this system in the k_y plane. In addition, we can derive the density of states (DOS) represented by $D(E)$ and given by

$$D(E) = \sum_{n, k_y} \delta(E - E_{n, k_y}), \quad (19)$$

and expressed in units of $D_0 = L/\hbar v_F$, which corresponds to the amount of states per unit area and L is the period of the superlattice.

IV. PRISTINE SYSTEM

To start, we consider the pristine system corresponding to $\hat{U}_i = 0$ in Eq. (10). The solution of $\hat{H}\Psi_j = E\Psi_j$ in this case leads to $\alpha_j = \gamma_j = \beta_j = 1$ in the wave-functions given by Eq. (11). Moreover, from the secular equation $\det(\hat{H} - E) = 0$ we obtain, respectively, the wave-vectors in the x -direction in the well and barrier regions

$$k_w = \sqrt{\left(\frac{E}{\hbar v_F}\right)^2 - k_y^2}, \quad k_b = \sqrt{\left(\frac{E - V_b}{\hbar v_F}\right)^2 - k_y^2}, \quad (20)$$

with $\hbar v_F = 3a_0 t/2$.

From the transfer matrix in Eq. (16) we find the dispersion relation given by Eq. (18) with $G_U = G_0$ where

$$G_0 = \frac{1}{k_w k_b} \left[\frac{E(E - V_b)}{\hbar^2 v_F^2} + \frac{(E^2 + (E - V_b)^2) k_y^2 (\cos^2(2\theta) - 1)}{2E(E - V_b)} - k_y^2 \cos^2(2\theta) \right]. \quad (21)$$

An electrostatic superlattice is capable of multiplying the number of Dirac points²¹. These are points in reciprocal space where the valence and conduction bands

touch each other and around which the energy spectrum is linear. Therefore, it is interesting to calculate how the $\alpha - T_3$ lattice Dirac point is affected by the superlattice

potential.

In order to determine the location of the Dirac points for the symmetric case $W_b = W_w = W$ we take $K_x = 0$, and $k_b = k_w$ in Eq. (18). Inserting this latter condition into Eq. (20), we have $E = V_b/2$. Thus, Eq. (18) becomes

$$1 = \cos^2(k_b W) + \sin^2(k_b W) \left[\frac{V_0^2/4\hbar^2 v_F^2 + 2k_y^2 \cos^2(2\theta) - k_y^2}{V_0^2/4\hbar^2 v_F^2 - k_y^2} \right]. \quad (22)$$

This equation has solutions when the term between brackets is equal to 1, or $\sin^2(k_b W) = 1$. The first possibility is obtained for $k_y = 0$ and corresponds to the main Dirac point at $k_y = 0$. The second possibility leads to $k_b W = n\pi$ with n being a positive integer. This last possibility determines the position of the extra Dirac points in k_y space from Eq. (20),

$$k_y = \sqrt{\frac{V_b^2}{4\hbar^2 v_F^2} - \left(\frac{n\pi}{W}\right)^2}. \quad (23)$$

Note from Eq. (22) that for the symmetric case the condition to determine the position of Dirac points is regardless of the parameter θ . Note that when $\theta = 0$, Eq. (22) reduces to

$$1 = \cos^2(k_b W) + \sin^2(k_b W) \left[\frac{(V_b^2/4\hbar^2 v_F^2 + k_y^2)}{(V_b^2/4\hbar^2 v_F^2 - k_y^2)} \right], \quad (24)$$

which is consistent with the equation that determines the Dirac points for graphene²¹. As discussed above, there is no real solution for Eq. (24) unless $k_y = 0$ that represents the usual Dirac point, or $k_b W = n\pi$ ^{18,21,22}.

On the other hand, when we set $\theta = \pi/4$, Eq. (22) leads to

$$\cos^2(k_b W) + \sin^2(k_b W) = 1. \quad (25)$$

Unlike the graphene-like case, Eq. (22) has many solutions and the condition for allowed states in the dispersion relation of Eq. (18) is always satisfied for arbitrary k_y .

In Figs. 6(a-d) we show the electronic band structures at $K_x L = 0$ for some values of the parameter θ assuming $W_w = W_b = L/2$ and $V_b = 7E_L$, where $E_L = \hbar v_F/L$ and $L/a_0 = 1200$. As discussed above, one Dirac point appears at $E = V_b/2$ and $k_y L = 0$ for $0 \leq \theta < \pi/4$ as shown in Figs. 6(a-c), moreover the upper and lower bands gradually becomes closer as the structure reaches $\theta = \pi/4$ (dice lattice), when the Dirac point disappears and all states at $E = 3.5E_L$ are allowed regardless of the values of $k_y L$, as shown in Fig. 6(d).

The dependence on the parameter θ observed in the energy spectra can be better understood from the density of states (DOS) shown in Fig. 7 for the same parameters as in Fig. 6. For the dice case, depicted by the magenta dotted curve, we notice the presence of a pronounced peak,

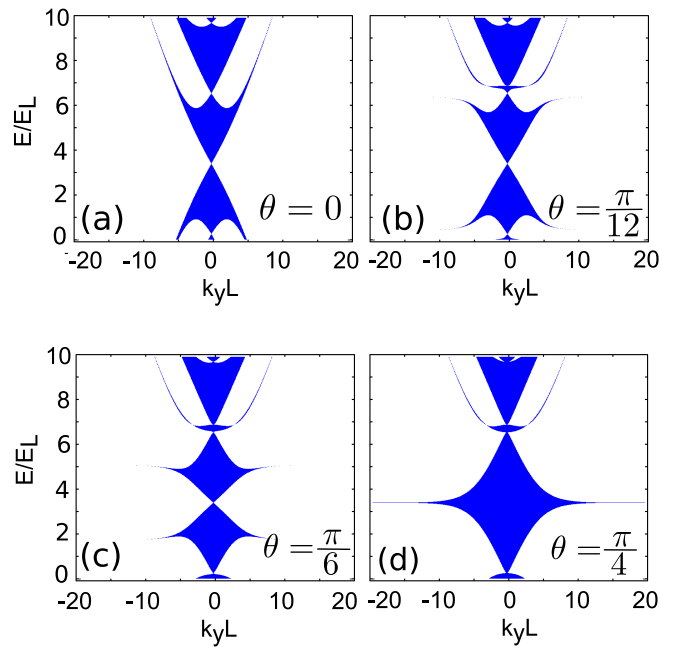


FIG. 6: Electronic band structures at $K_x L = 0$ for (a) $\theta = 0$ (graphene-like case), (b) $\theta = \pi/12$, (c) $\theta = \pi/6$, (d) $\theta = \pi/4$ (dice case) with $V_b = 7E_L$, $W_w = W_b = L/2$, where $L/a_0 = 1200$, and $E_L = \hbar v_F/L$

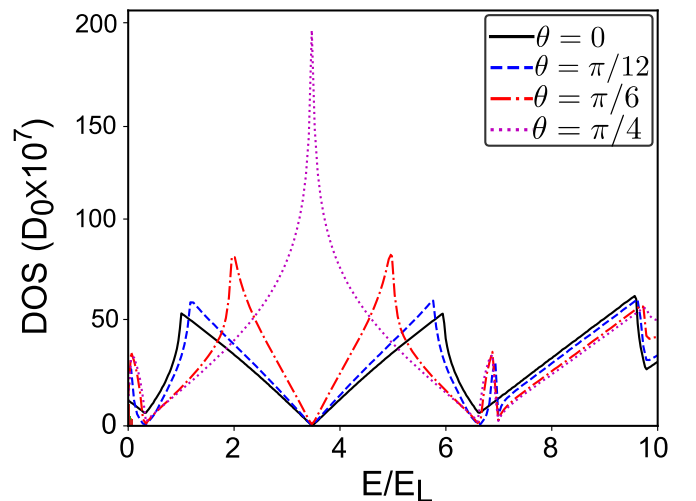


FIG. 7: Density of states for $\theta = 0$ (black solid curve), $\theta = \pi/12$ (blue dashed curve), $\theta = \pi/6$ (red dash-dotted curve), $\theta = \pi/4$ (magenta dotted curve) for the same parameters as in Fig. 6.

which agrees with Eq. (25) representing the manifestation of the flat band and, therefore, an enhancement of the number of states.

In Fig. 8 the spectrum resulting from Eq. (18) using Eq. (21) for equal barrier and well width is plotted taking $L/a_0 = 1200$, and $V_b = 21E_L$ for $\theta = 0$ and $\theta = \pi/4$. We observe for the honeycomb case, i.e. $\theta = 0$, the appearance of extra Dirac points localized to the left and to

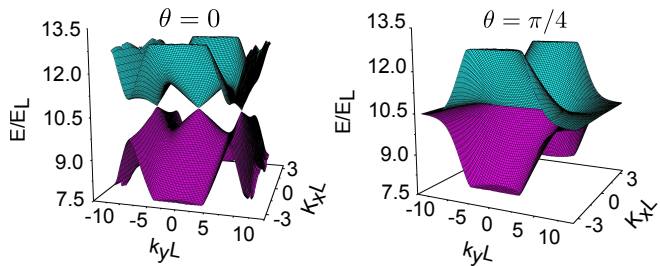


FIG. 8: Valence and conduction bands of the spectrum of a superlattice considering $\theta = 0$ (graphene-like), and $\theta = \pi/4$ (dice) with $V_b = 21E_L$, $W_w = W_b = L/2$, where $L/a_0 = 1200$, and $E_L = \hbar v_F/L$.

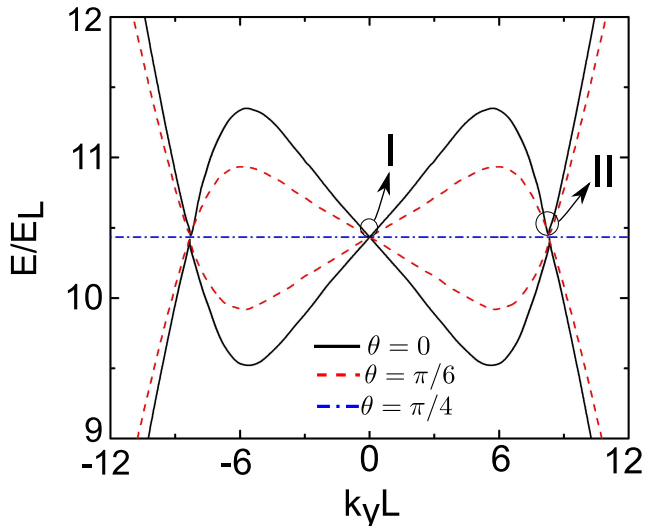


FIG. 9: Electronic band structures for $K_x L = 0$ with $\theta = 0$ (black solid curve), $\theta = \pi/6$ (red dashed curve), and $\theta = \pi/4$ (blue dot-dashed curve) for $K_x L = 0$ with $V_b = 21E_L$, $W_w = W_b = L/2$, where $L/a_0 = 1200$, and $E_L = \hbar v_F/L$.

the right of the main one at the energy corresponding to $V_b = 10.5E_L$ for $K_x L = 0$. However, at this same point for the dice case the Dirac points disappear giving rise to a flat band, which can be observed clearer in Fig. 9 where we show the superlattice spectrum along $k_y L$ for $K_x L = 0$ for different values of θ . We notice that as θ increases the spacing between the upper and lower bands around the Dirac points decreases.

Moreover, the group velocity along the $k_y L$ direction around the main and the extra Dirac points denoted in Fig. 9 by the labels *I* and *II* is shown in Fig. 10. Notice that the slope of the dispersion relation around these

points is strongly reduced as compared to the value v_F when no superlattice is imposed. This result is similar to the collimation effect observed in graphene as new extra Dirac points are to arise when the height of the potential V_b increases as discussed in Ref. 21. But now, the collimation effect results from changing the coupling constant θ .

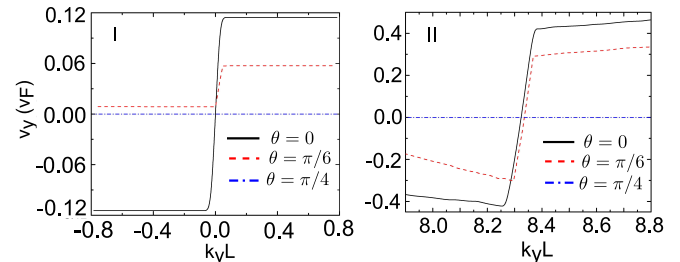


FIG. 10: Group velocity along k_y direction around the main Dirac point (I), and around the extra Dirac point (II) indicated in Fig. 9.

V. INTRODUCTION OF GAPS IN THE SUPERLATTICE ENERGY SPECTRUM

Using the transfer matrix formalism from Sec. III, we analyze the appearance and morphing in $\alpha - T_3$ superlattices when including deviations in the atomic equivalence of the three sublattices and by adding the terms \hat{U}_1 or \hat{U}_2 .

A. Case $\hat{U} = \hat{U}_1$

Assuming $\hat{U} = \hat{U}_1$ in Eq. (10), we obtain the wavefunctions expressed in Eq. (11) in the well ($j = w$) and barrier ($j = b$) with $\alpha_w = \beta_w = \sqrt{E + \Delta}$, $\alpha_b = \beta_b = \sqrt{E - V_b + \Delta}$, $\gamma_w = \sqrt{E - \Delta}$ and $\gamma_b = \sqrt{E - V_b - \Delta}$.

The wave-vectors in x -direction in the well and barrier regions are

$$k_w = \sqrt{\frac{E^2 - \Delta^2}{\hbar^2 v_F^2} - k_y^2}, \quad (26a)$$

$$k_b = \sqrt{\frac{(E - V_b)^2 - \Delta^2}{\hbar^2 v_F^2} - k_y^2}. \quad (26b)$$

From the transfer matrix method we get the dispersion relation in Eq.(18) with $G_U = G_1$

$$G_1 = -\frac{1}{2} \left[\left(\frac{\eta_{w1}}{\eta_{b1}} + \frac{\eta_{b1}}{\eta_{w1}} \right) + \cos^2(2\theta) \left(\frac{k_y^2}{k_b^2} \frac{\eta_{b1}}{\eta_{w1}} + \frac{k_y^2}{k_w^2} \frac{\eta_{w1}}{\eta_{b1}} \right) - 2 \frac{k_y^2}{k_w k_b} \cos^2(2\theta) \right], \quad (27)$$

with $\eta_{w_1} = k_w \hbar v_F / (E - \Delta)$ and $\eta_{b_1} = k_b \hbar v_F / (E - V_b - \Delta)$.

In order to analyze the effects on the energy spectrum, and investigate how the Dirac points are affected due to the presence of this symmetry-breaking term, we consider $W_b = W_w = W$, and $k_w W = -k_b W$ in Eq. (18) at the energy $E = V_b/2$ where, for gap-less case, the Dirac points are found. When we take into account these considerations and we assume $\theta = 0$, the dispersion relation becomes

$$\cos(K_x L) = \cos^2(k_b W) + \sin^2(k_b W) \left[\frac{(V_b^2/4 + \Delta^2)/\hbar^2 v_F^2 + k_y^2}{(V_b^2/4 - \Delta^2)/\hbar^2 v_F^2 - k_y^2} \right], \quad (28)$$

which has no real solution regardless of the value of k_y , indicating the presence of a band gap in the energy spectrum. This result can be extended to other cases where $\cos 2\theta \neq 0$ in Eq. (27).

Assuming the particular case $\theta = \pi/4$ we get

$$\cos(K_x L) = \cos^2(k_b W) + \sin^2(k_b W) \left[\frac{(V_b^2/4 + \Delta^2)/\hbar^2 v_F^2 - k_y^2 ((V_b^2/4 + \Delta^2)/(V_b^2/4 - \Delta^2))}{(V_b^2/4 - \Delta^2)/\hbar^2 v_F^2 - k_y^2} \right], \quad (29)$$

which has a real solution for two touching points $k_y = \pm \sqrt{V_b^2/4 - \Delta^2}/\hbar v_F$. Unlike the dice case in the absence of a mass term discussed in Sec. III, the energy allowed states in the presence of a symmetry-breaking term is no longer independent of k_y at $E = V_b/2$.

This becomes more clear when we calculate the electronic band structure for some particular values of the parameter θ , the effective mass term $\Delta = 0.1V_b$, $V_b = 7E_L$, and $L/a_0 = 1200$. The results are depicted in Fig. 11, where $E_L = \hbar v_F/L$. As discussed from Eq. (28) and Eq. (29), we can observe the presence of a band gap in the energy spectra at $E = V_b/2$, or, in terms of the unit E_L , $E \approx 3.5E_L$. Except for $\theta = \pi/4$, where the band gap is closed at the touching points $k_y = \pm \sqrt{V_b^2/4 - \Delta^2}/\hbar v_F$, but we observe the formation of another band gap at energy $E \approx 5E_L$. Moreover, the mini-bands present in the energy spectra for intermediate values of θ are no longer symmetric around the band gap, as shown in Figs. 11(b)-(c). The band gap morphing and its dependence on θ can be observed when we analyze the density of states (DOS) of those systems shown in Fig. 12. The appearance of asymmetric mini-bands, and the band gap shifting observed in Fig. 11(d) becomes clearly apparent. In addition, unlike the graphene-like case, when we assume $\theta \neq 0$ a new allowed energy state arises which appears as a new peak localized in the energy range $7E_L$ to $8E_L$ as observed in Fig. 12.

On the other hand, when we take a large value for the mass term $\Delta = 0.4V_b$ maintaining the other parameters used in Fig. 11, beyond the increased gap, we found that the mini-bands change drastically. When $\theta \neq 0$, the energy spectra exhibit significant modifications in a large

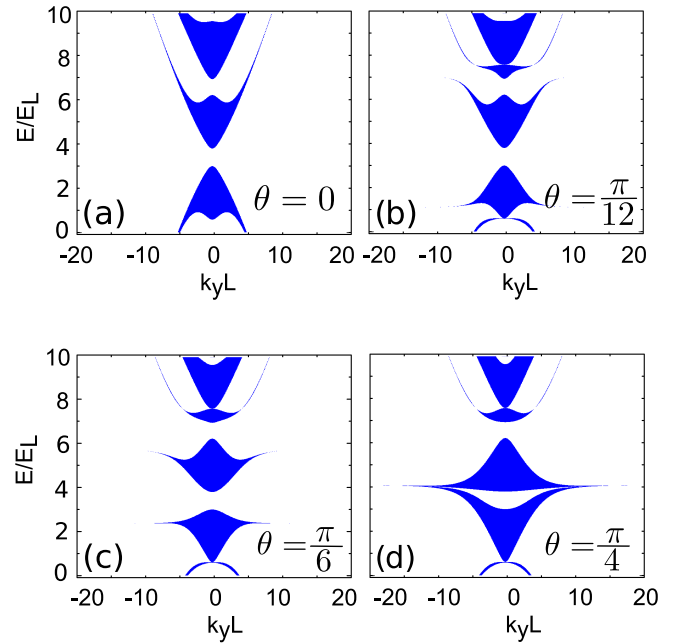


FIG. 11: Electronic band structures at $K_x L = 0$ for (a) $\theta = 0$ (graphene-like case), (b) $\theta = \pi/12$, (c) $\theta = \pi/6$, (d) $\theta = \pi/4$ (dice case) with $V_b = 7E_L$, $W_w = W_b = L/2$, $\Delta = 0.1V_b$ and $\hat{U} = \hat{U}_1$, where $L/a_0 = 1200$, and $E_L = \hbar v_F/L$ in all cases.

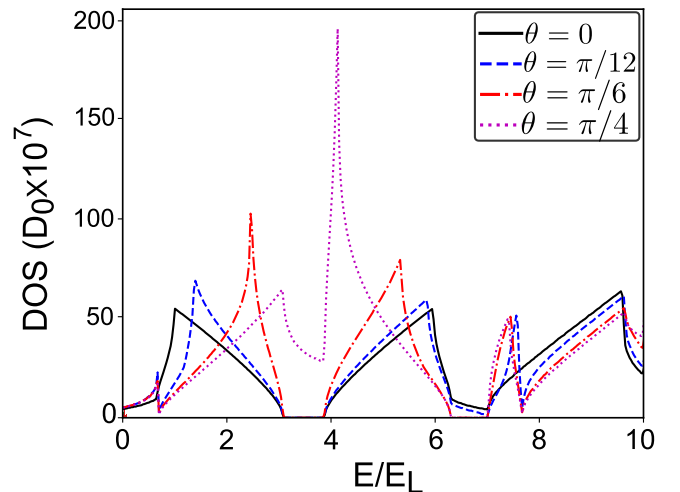


FIG. 12: Density of states for $\theta = 0$ (black solid curve), $\theta = \pi/12$ (blue dashed curve), $\theta = \pi/6$ (red dash-dotted curve), $\theta = \pi/4$ (magenta dotted curve) for the same parameters as in Fig. 11.

range of energy, as shown in Figs. 13(b)-(d), where it is possible to see the appearance of new mini-bands inside the band gap region, unlike the graphene-like case. The appearance of new allowed states inside the region where for the graphene-like case there is only a band gap, is clearly seen from the density of states, as shown in Fig. 14. In addition, the position of the touching points given by $k_y = \pm \sqrt{V_b^2/4 - \Delta^2}/\hbar v_F$ depends on the mass

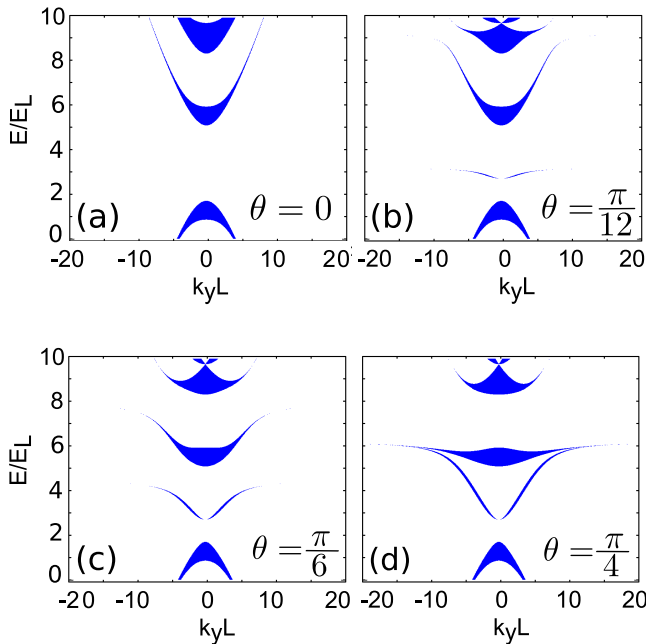


FIG. 13: Electronic band structures at $K_x L = 0$ for (a) $\theta = 0$ (graphene-like case), (b) $\theta = \pi/12$, (c) $\theta = \pi/6$, (d) $\theta = \pi/4$ (dice case) with $V_b = 7E_L$, $W_w = W_b = L/2$, $\Delta = 0.4V_b$ for $\hat{U} = \hat{U}_1$, where $L/a_0 = 1200$, and $E_L = \hbar v_F/L$ in all cases.

term value, and these points are shifted, as shown in Fig. 13(d). From Fig. 14 we observe that there is a

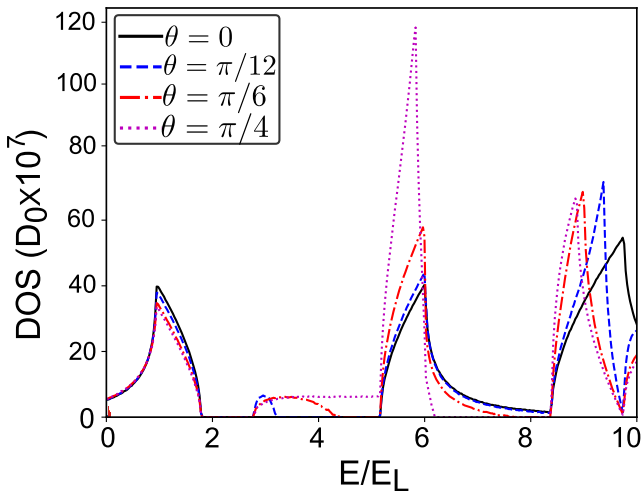


FIG. 14: Density of states for $\theta = 0$ (black solid curve), $\theta = \pi/12$ (blue dashed curve), $\theta = \pi/6$ (red dash-dotted curve), $\theta = \pi/4$ (magenta dotted curve) for the same parameters as in Fig. 13.

prominent peak when the dice case is considered similar to Fig. 12 but localized at different energy, which results from the increase of the mass term Δ . Moreover, it is evident that there are more allowed states in the energy range $2E_L$ to $5E_L$ for $\theta \neq 0$.

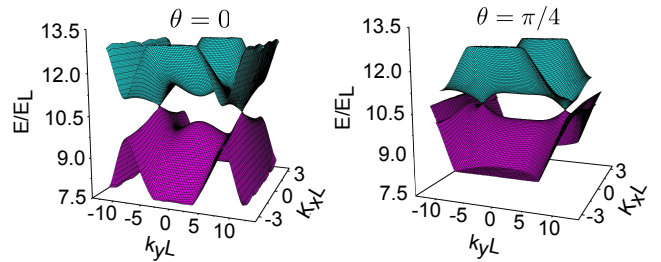


FIG. 15: Valence and conduction bands of the spectrum of a superlattice considering $\theta = 0$ (graphene-like), and $\theta = \pi/4$ (dice) with $V_b = 21E_L$, $W_w = W_b = L/2$, $\hat{U} = \hat{U}_1$, and $\Delta = 0.4V_b$. Where $L/a_0 = 1200$, and $E_L = \hbar v_F/L$.

In Fig. 15 we show the dispersion relation obtained from Eq. (21) and Eq. (27) assuming equal barrier and well widths, $L/a_0 = 1200$, $V_b = 21E_L$, and $\Delta = 0.4V_b$ for $\theta = 0$ and $\theta = \pi/4$. Unlike the gap-less case, for $\theta = 0$ the main Dirac point at $k_y L = 0$ is no longer observed, although the extra Dirac points on both sides remains. Similarly, for the dice case, the upper and lower mini-bands touch each other at two-points $k_y L \neq 0$, similar as in Fig. 11(d) and Fig. 13(d).

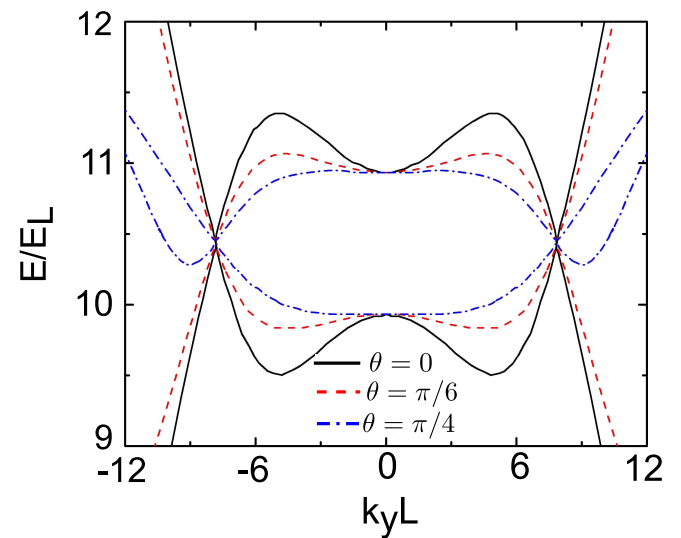


FIG. 16: Electronic band structures at $K_x L = 0$ for $\theta = 0$ (black solid curve), $\theta = \pi/6$ (red dashed curve), and $\theta = \pi/4$ (blue dot-dashed curve) with $V_b = 21E_L$, $W_w = W_b = L/2$, $\Delta = 0.4V_b$ where $L/a_0 = 1200$, and $E_L = \hbar v_F/L$.

Moreover, when we assume the superlattice spectrum along $k_y L$ direction for $K_x L = 0$ in Fig. 15 we find that the dispersion gradually changes around the point $k_y L = 0$, becoming flat for $\theta = \pi/4$, as shown in Fig. 16. In addition, around the touching points the slope of the dispersion decreases as θ increases.

B. Case $\hat{U} = \hat{U}_2$

For the other symmetry-breaking term denoted by $\hat{U} = \hat{U}_2$ in Eq. (10), we have $\alpha_w = \sqrt{1 + 2\Delta/(E - \Delta)}$, $\alpha_b = \sqrt{1 + 2\Delta/(E - V_b - \Delta)}$, $\gamma_w = \sqrt{1 + \Delta \cos(2\theta)/E}$, $\gamma_b = \sqrt{1 + \Delta \cos(2\theta)/(E - V_b)}$, $\beta_w = \sqrt{1 - 2\Delta/(E + \Delta)}$, and $\beta_b = \sqrt{1 - 2\Delta/(E - V_b + \Delta)}$. Consequently, the wavefunctions k_w and k_b are given by

$$k_w = \sqrt{\frac{(E^2 - \Delta^2)E}{(\hbar^2 v_F^2)(E + \Delta \cos 2\theta)}} - k_y^2, \quad (30a)$$

$$k_b = \sqrt{\frac{((E - V_b)^2 - \Delta^2)(E - V_b)}{(\hbar^2 v_F^2)(E - V_b + \Delta \cos 2\theta)}} - k_y^2. \quad (30b)$$

For this case we have

$$G_2 = -\frac{1}{2} \left[\left(\frac{\eta_{w_2}}{\eta_{b_2}} + \frac{\eta_{b_2}}{\eta_{w_2}} \right) + \left(\frac{k_y^2 \eta_{b_2}}{k_b^2 \eta_{w_2}} \frac{((E - V_b) \cos 2\theta + \Delta)^2}{(E - V_b + \Delta \cos 2\theta)^2} + \frac{k_y^2 \eta_{w_2}}{k_w^2 \eta_{b_2}} \frac{(E \cos 2\theta + \Delta)^2}{(E + \Delta \cos 2\theta)^2} \right) - \frac{2k_y^2}{k_w k_b} \frac{((E - V_b) \cos 2\theta + \Delta)(E \cos 2\theta + \Delta)}{(E - V_b + \Delta \cos 2\theta)(E + \Delta \cos 2\theta)} \right], \quad (31)$$

and

$$\eta_{w_2} = \frac{k_w}{(E^2 - \Delta^2)(E + \Delta \cos 2\theta)}, \quad (32a)$$

$$\eta_{b_2} = \frac{k_b}{[(E - V_b)^2 - \Delta^2][(E - V_b) + \Delta \cos 2\theta]}. \quad (32b)$$

From Eq. (10) assuming $\Delta = 0.1V_b$ for $\hat{U} = \hat{U}_2$, and the same values of L and V_b as in Fig. 6, we get the energy spectra shown in Fig. 17 for different values of θ . Similar to the case $\hat{U} = \hat{U}_1$ we observe the presence of a band gap for all values of $\theta \neq \pi/4$ around $E = V_b/2$, i.e $E = 3.5E_L$, and the mini-bands tend to reach each other around this energy as θ increases until the band gap is completely closed for the dice case, as shown in Fig. 17(d). Like the gapless case, all energy states when $\theta = \pi/4$ are allowed regardless of the k_y value, which results in a prominent peak in the density of states depicted in Fig. 18. This result can be expected when we assume the condition $W_b = W_w = W$, $E = V_b/2$, and $\theta = \pi/4$ in the dispersion relation for this case. Under these conditions, the dispersion relation for the dice lattice reduces to the same one for the gapless case represented in Eq. (25).

Moreover, comparing the band gap width observed in Fig. 17 to the one in Fig. 11 the band gap is reduced and shifted up, as observed in Fig. 18.

Similar to the previous gapped case, if we consider a larger value of the mass term $\Delta = 0.4V_b$ the band gap is increased and other allowed states appear inside them when intermediate values of θ are considered, as shown in Fig. 19. However the allowed state for arbitrary values of k_y at $E = V_b/2$ for the dice lattice is preserved and a peak in the density of states is observed for $\theta = \pi/4$, as shown in Fig. 20, since this condition is independent of

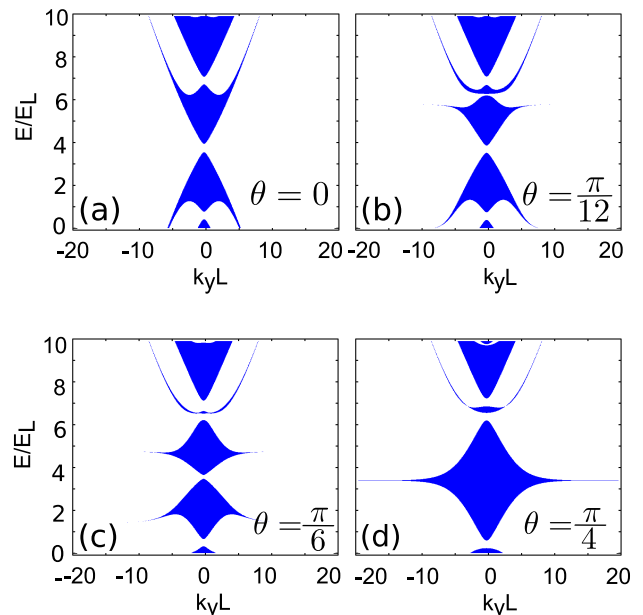


FIG. 17: Electronic band structures at $K_x L = 0$ for (a) $\theta = 0$ (graphene-like case), (b) $\theta = \pi/12$, (c) $\theta = \pi/6$, (d) $\theta = \pi/4$ (dice case) with $V_b = 7E_L$, $W_w = W_b = L/2$, $\Delta = 0.1V_b$ when $\hat{U} = \hat{U}_2$, where $L/a_0 = 1200$, and $E_L = \hbar v_F/L$ in all cases.

the value of the effective mass. The spectrum obtained from Eq. (18) and Eq. (31) considering equal barrier and well widths, $L/a_0 = 1200$, $V_b = 21E_L$, and $\Delta = 0.4V_b$ for $\theta = 0$ and $\theta = \pi/4$ are shown in Fig. 21. Similar to previous gapped case, for $\theta = 0$ the upper and lower mini-bands touch each other in two-points, and at $k_y L = 0$ there is a gap. However, as discussed above, the energy where the touching points are localized is no longer at

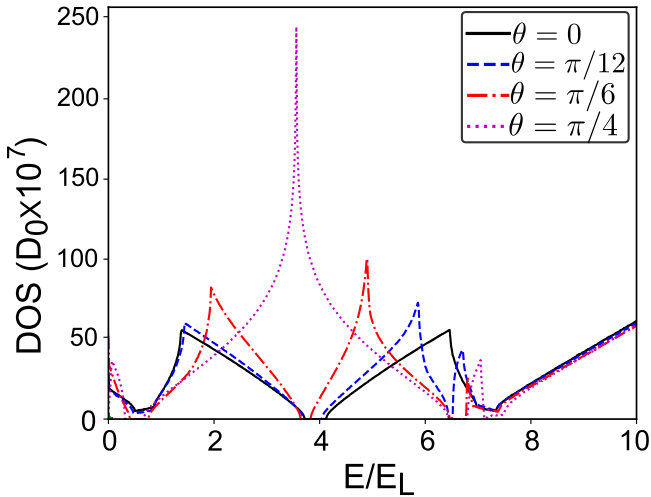


FIG. 18: Density of states for $\theta = 0$ (black solid curve), $\theta = \pi/12$ (blue dashed curve), $\theta = \pi/6$ (red dash-dotted curve), $\theta = \pi/4$ (magenta dotted curve) for the same parameters as in Fig. 17.

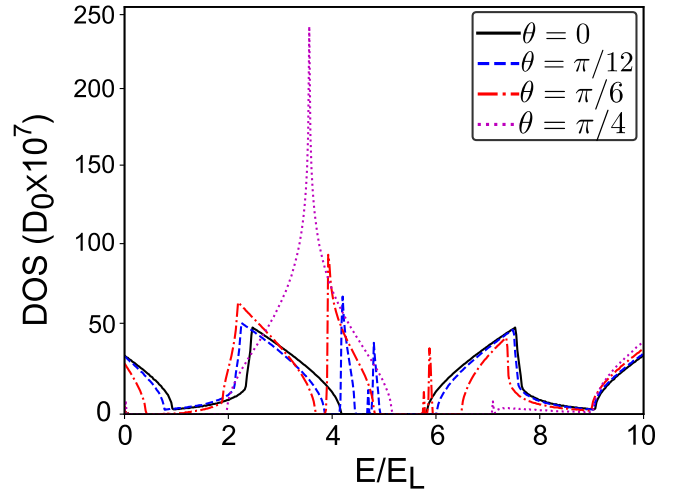


FIG. 20: Density of states for $\theta = 0$ (black solid curve), $\theta = \pi/12$ (blue dashed curve), $\theta = \pi/6$ (red dash-dotted curve), $\theta = \pi/4$ (magenta dotted curve) for the same parameters as in Fig. 19.

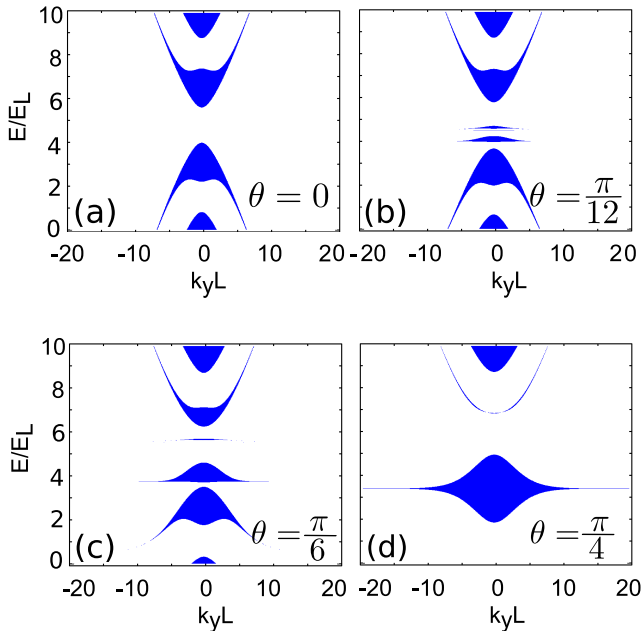


FIG. 19: Electronic band structures at $K_x L = 0$ for (a) $\theta = 0$ (graphene-like case), (b) $\theta = \pi/12$, (c) $\theta = \pi/6$, (d) $\theta = \pi/4$ (dice lattice) with $V_b = 7E_L$, $W_w = W_b = L/2$, $\Delta = 0.4V_b$ when $\hat{U} = \hat{U}_2$, where $L = 1200$, and $E_L = \hbar v_F/L$ in all cases.

$E = V_b/2$. On the other hand, for the dice lattice the spectrum is completely flat at $k_y L = 0$ and $E = V_b/2$, similar to Fig. 8.

In Fig. 22 we show the superlattice spectrum considering $K_x L = 0$ along $k_y L$ direction for some values of θ . Notice that the energy where the touching points are localized depends on θ . Moreover, like the gapless case, as $\theta \rightarrow \pi/4$ the dispersion becomes flat and shifted to

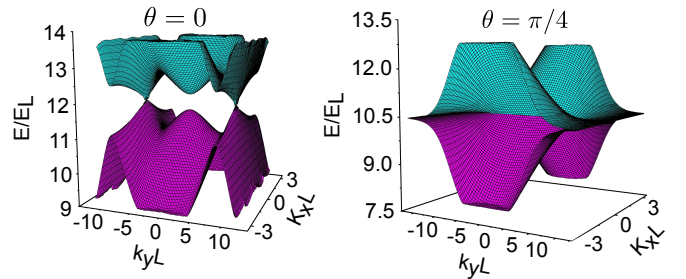


FIG. 21: Valence and conduction bands of the spectrum of a superlattice considering $\theta = 0$ (graphene-like), and $\theta = \pi/4$ (dice) with $V_b = 21E_L$, $W_w = W_b = L/2$, $\hat{U} = \hat{U}_2$, and $\Delta = 0.4V_b$. Where $L/a_0 = 1200$, and $E_L = \hbar v_F/L$.

lower values of energy.

VI. CONCLUSIONS

We investigated the energy spectrum and the density of states (DOS) of $\alpha - T_3$ lattices for different values of interlattice hopping parameter $\theta = \tan^{-1} \alpha$ in the presence of a 1D superlattice. We consider both the case of equivalence between the three sub-lattices, and how the band gap is affected by small deviations of this equivalence in the limit $\Delta \ll t$ by considering two cases of symmetry-breaking terms denoted by \hat{U}_1 and \hat{U}_2 .

For the pristine system, when no symmetry-breaking term are present, we found the condition for the appearance of Dirac points that depends on the cosine function of the parameter θ , indicating that the energy level where they are located remains the same for all cases when $\cos(2\theta) \neq 1$. When $\theta = \pi/4$ all energies are allowed for arbitrary k_y . Moreover, the mini-bands for in-

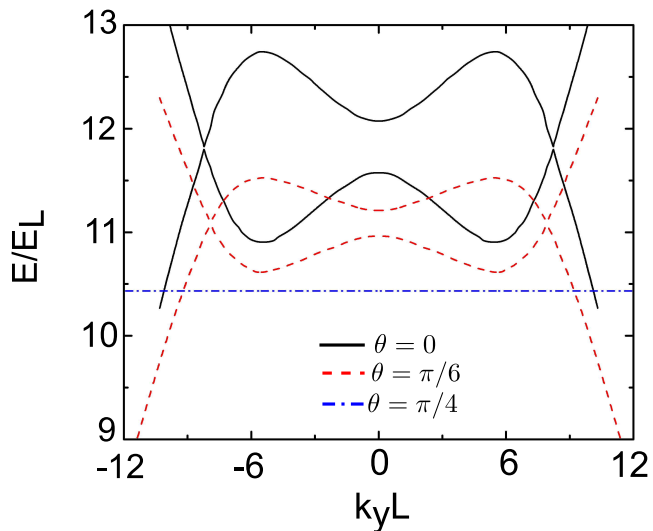


FIG. 22: Electronic band structures at $K_x L = 0$ for $\theta = 0$ (black solid curve), $\theta = \pi/6$ (red dashed curve), and $\theta = \pi/4$ (blue dot-dashed curve) with $V_b = 21E_L$, $W_w = W_b = L/2$, $\Delta = 0.4V_b$ where $L/a_0 = 1200$, and $E_L = \hbar v_F/L$.

intermediate values of θ tends to close around the energy level where Dirac points are localized. In addition, when we considered higher values of the potential, we observed extra Dirac points localized on the right and on the left of the main one positioned at $k_y = 0$ for all values of $\theta \neq \pi/4$.

When we introduce symmetry-breaking terms into the system, we observed the appearance of a band gap, whose creation depends on the deviation on the equivalence between the three sub-lattices. When we considered the case $\hat{U}_1 = \text{diag}(1, -1, 1)$, a band gap appears at energy $E = V_b/2$. However for the dice case, around this energy, there is no longer a band gap and the mini-bands touch at two points. This result can be observed either in the energy spectra and in their corresponding DOS.

In addition, the mini-bands for larger values of the mass term was shifted up, which is a consequence of the fact that the sites A and C remain equivalent, leading to twofold degeneracy of the energy spectra, as in the case when there is no periodic potential present. Moreover, for larger values of the potential the main Dirac point for all θ values is no longer present, only the extra ones appear and are localized at the energy $E = V_b/2$.

When $\hat{U}_2 = \text{diag}(1, 0, -1)$, the dispersion relation, and consequently, the energy spectrum is strongly altered. For the dice case, we found that the condition for the allowance of the energy states at $E = V_b/2$ is always satisfied regardless of k_y , similarly as in the gapless case. However a band gap is still present but now localized at another energy. In addition, we noticed that the band gap is smaller than the one observed when \hat{U}_1 . Moreover, for larger values of the effective mass new energy states were observed inside the band gap as confirmed from the density of states. In addition, for higher values of the

potential considering $\theta \neq \pi/4$ only the extra Dirac points are observed, like for the previous gapped case, but now the energy value where they are localized depends on the hopping parameter.

The theoretical formalism and results obtained in this work are useful for a better understanding of the band-gap behaviour of $\alpha - T_3$ lattices, and consequently demonstrate that these materials are versatile for purposes of band-gap engineering in 2D materials, since the band-gap is tunable by changing the interlattice hopping parameter and their symmetry.

VII. ACKNOWLEDGMENTS

This study was financed in part by the Coordenação de Aperfeiçoamento de Pessoal de Nível Superior-Brasil (CAPES)-Finance code 88887.508174/2020 – 00, and the Flemish Science Foundation (FWO-V1) through a postdoc fellowship for B.V.D.

* Electronic address: sofiacunha@fisica.ufc.br

† Electronic address: ben.vanduppen@uantwerpen.be

- ¹ K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, Y. Zhang, S. V. Dubonos, I. V. Grigorieva, and A. A. Firsov, Electric field effect in atomically thin carbon films, *Science* **306**, 666 (2004).
- ² S. V. Morozov, K. S. Novoselov, M. I. Katsnelson, F. Schedin, D. C. Elias, J. A. Jaszczak, and A. K. Geim, Giant Intrinsic Carrier Mobilities in Graphene and Its Bilayer, *Phys. Rev. Lett.* **100**, 016602 (2008).
- ³ M. I. Katsnelson, K. S. Novoselov, and A. K. Geim, Chiral tunnelling and the Klein paradox in graphene. *Nature Phys.* **2**, 620625 (2006).
- ⁴ E. B. Sonin, Effect of Klein tunneling on conductance and shot noise in ballistic graphene, *Phys. Rev. B* **79**, 195438 (2009).
- ⁵ Han Liu, Adam T. Neal, Zhen Zhu, Zhe Luo, Xianfan Xu, David Tománe, and Peide D. Ye, Phosphorene: An Unexplored 2D Semiconductor with a High Hole Mobility, *ACS Nano*. **8**, 4033-4041, (2014).
- ⁶ Cheng-Cheng Liu, Hua Jiang, and Yugui Yao, Low-energy effective Hamiltonian involving spin-orbit coupling in silicene and two-dimensional germanium and tin, *Phys. Rev. B* **84**, 195430 (2011).
- ⁷ M. E. Dávila, L. Xian, S. Cahangirov, A. Rubio, and G. Le. Lay, Germanene: a novel two-dimensional germanium allotrope akin to graphene and silicene, *New J. Phys.* **16**, 095002 (2014).
- ⁸ D. P. DiVincenzo and E. J. Mele, Self-consistent effective-mass theory for intralayer screening in graphite intercalation compounds, *Phys. Rev. B* **29**, 1685
- ⁹ N. M. R Peres, Scattering in one-dimensional heterostructures described by the Dirac equation, *J. Phys.: Condens. Matter* **21**, 095501 (2009).
- ¹⁰ N. Stander, B. Huard, and D. Goldhaber-Gordon, Evidence for Klein Tunneling in Graphene pn Junctions, *Phys. Rev. Lett.* **102**, 026807 (2009).
- ¹¹ A. Young and P. Kim, Quantum interference and Klein tunnelling in graphene heterojunctions, *Nature Phys.* **5**, 222226 (2009).
- ¹² B. Huard, J. A. Sulpizio, N. Stander, K. Todd, B. Yang, and D. Goldhaber-Gordon, Transport Measurements Across a Tunable Potential Barrier in Graphene, *Phys. Rev. Lett.* **98**, 236803 (2007).
- ¹³ P. E. Allain and J. N. Fuchs, Klein tunneling in graphene: optics with massless electrons. *Eur. Phys. J. B* **83**, 301 (2011).
- ¹⁴ R. Tsu, *Superlattice to Nanoelectronics* (Elsevier, Oxford, 2005).
- ¹⁵ Chunxu Bai and Xiangdong Zhang, Klein paradox and resonant tunneling in a graphene superlattice, *Phys. Rev. B* **76**, 075430 (2007).
- ¹⁶ C. H. Park, L. Yang, Y. W. Son, M. L. Cohen, and Steve G. Louie, Anisotropic behaviours of massless Dirac fermions in graphene under periodic potentials, *Nature Phys.* **4**, 213217 (2008).
- ¹⁷ Michaël Barbier, F. M. Peeters, P. Vasilopoulos, and J. Milton Pereira, Jr., Dirac and Klein-Gordon particles in one-dimensional periodic potentials, *Phys. Rev. B* **77**, 115446 (2008).
- ¹⁸ Li-Gang Wang and Shi-Yao Zhu, Electronic band gaps and transport properties in graphene superlattices with one-dimensional periodic potentials of square barriers, *Phys. Rev. B* **81**, 205444 (2010).
- ¹⁹ Jianmin Sun, H. A. Fertig, and L. Brey, Effective Magnetic Fields in Graphene Superlattices, *Phys. Rev. Lett.* **105**, 156801 (2010).
- ²⁰ Liang Zheng Tan, Cheol-Hwan Park, and Steven G. Louie, Graphene Dirac fermions in one-dimensional inhomogeneous field profiles: Transforming magnetic to electric field, *Phys. Rev. B* **81**, 195426 (2010).
- ²¹ M. Barbier, P. Vasilopoulos, and F. M. Peeters, Extra Dirac points in the energy spectrum for superlattices on single-layer graphene, *Phys. Rev. B* **81**, 075438 (2010).
- ²² L. Brey and H. A. Fertig, Emerging Zero Modes for Graphene in a Periodic Potential, *Phys. Rev. Lett.* **103**, 046809 (2009).
- ²³ Cheol-Hwan Park, Young-Woo Son, Li Yang, Marvin L. Cohen, and Steven G. Louie, Landau Levels and Quantum Hall Effect in Graphene Superlattices, *Phys. Rev. Lett.* **103**, 046808 (2009).
- ²⁴ Michaël Barbier, P. Vasilopoulos, and F. M. Peeters, Single-layer and bilayer graphene superlattices: collimation, additional Dirac points and Dirac lines, *Phil. Trans. R. Soc. A*. **368**: 54995524 (2010).
- ²⁵ Y. Li, S. Dietrich, C. Forsythe, T. Taniguchi, K. Watanabe, P. Moon, and C. R. Dean, Anisotropic band flattening in graphene with one-dimensional superlattices. *Nat. Nanotechnol.* **16**, 525530 (2021).
- ²⁶ C. H. Park, Y. W. Son, L. Yang, M. L. Cohen, and S. G. Louie, Electron Beam Supercollimation in Graphene Superlattices, *Nano Lett.* **8**, 2920 (2008).
- ²⁷ Sergey Borisenko, Quinn Gibson, Danil Evtushinsky, Volodymyr Zabolotnyy, Bernd Behner, and Robert J. Cava, Experimental Realization of a Three-Dimensional Dirac Semimetal, *Phys. Rev. Lett.* **113**, 027603 (2014)
- ²⁸ M. Slot, T. Gardenier, P. Jacobse, G.C.P. van Miert, S. N. Kempkes, S. J. M. Zevenhuizen, C. M. Smith, D. Vanmaekelbergh, and I. Swart, Experimental realization and characterization of an electronic Lieb lattice. *Nature Phys* **13**, 672676 (2017).
- ²⁹ Z. Li, J. Zhuang, L. Chen, L. Wang, H. Feng, X. Xu, X. Wang, C. Zhang, K. Wu, S. X. Dou, Z. Hu, and Y. Du, Realization of flat band with possible nontrivial topology in electronic Kagome lattice, arXiv:1708.04448.
- ³⁰ Z. K. Liu, B. Zhou, Y. Zhang, Z. J. Wang, H. M. Weng, D. Prabhakaran, S.-K. Mo, Z. X. Shen, Z. Fang, X. Dai, Z. Hussain, and Y. L. Chen, Discovery of a Three-Dimensional Topological Dirac Semimetal, *Na₃Bi*, *Science* **343**, 864-867 (2014)
- ³¹ Balázs Dóra, Janik Kailasvuori, and R. Moessner, Lattice generalization of the Dirac equation to general spin and the role of the flat band, *Phys. Rev. B* **84**, 195422 (2011)
- ³² A. Raoux, M. Morigi, J.-N. Fuchs, F. Piéchon, and G. Montambaux, From Dia- to Paramagnetic Orbital Susceptibility of Massless Fermions, *Phys. Rev. Lett.* **112**, 026402 (2014)
- ³³ Bill Sutherland, Localization of electronic wave functions due to local topology, *Phys. Rev. B* **34**, 5208 (1986)
- ³⁴ Elliott H. Lieb, Two theorems on the Hubbard model, *Phys. Rev. Lett.* **62**, 1201 (1989)
- ³⁵ J. D. Malcolm and E. J. Nicol, Magneto-optics of general

- pseudospins two-dimensional Dirac-Weyl fermions, *Phys. Rev. B* **90**, 035405 (2014)
- ³⁶ Z. Lan, N. Goldman, A. Bermudez, W. Lu, and P. Öhberg, Dirac-Weyl fermions with arbitrary spin in two-dimensional optical superlattices, *Phys. Rev. B* **84**, 165115 (2011)
- ³⁷ Luyang Wang and Dao-Xin Yao, Coexistence of spin-1 fermion and Dirac fermion on the triangular kagome lattice, *Phys. Rev. B* **98**, 161403(R) (2018)
- ³⁸ E. Illes, Properties of the $\alpha - T_3$ Model, Ph.D. thesis, University of Guelph, Canada, 2017.
- ³⁹ Andrii Iurov, Godfrey Gumbs, and Danhong Huang, Peculiar electronic states, symmetries, and Berry phases in irradiated $\alpha - T_3$ materials, *Phys. Rev. B* **99**, 205135 (2019).
- ⁴⁰ Yunkun Xie, Yaohua Tan, and Avik W. Ghosh, Spintronic signatures of Klein tunneling in topological insulators, *Phys. Rev. B* **96**, 205151 (2017).
- ⁴¹ Yafang Xu and Guojun Jin, Omnidirectional transmission and reflection of pseudospin-1 Dirac fermions in a Lieb superlattice, *Phys. Lett. A* **378**, 3554-3560 (2014).
- ⁴² Daniel F. Urban, Dario Bercioux, Michael Wimmer, and Wolfgang Häusler, Barrier transmission of Dirac-like pseudospin-one particles, *Phys. Rev. B* **84**, 115136 (2011).
- ⁴³ C.-Y. Tan, C.-X. Yan, Y.-H. Zhao, H. Guo, and H.-R. Chang, Anisotropic longitudinal optical conductivities of tilted Dirac bands in $1T' - MoS_2$, *Phys. Rev. B* **103**, 125425 (2021).
- ⁴⁴ Nicholas Weekes, Andrii Iurov, Liubov Zhemchuzhna, Godfrey Gumbs, and Danhong Huang, Generalized WKB theory for electron tunneling in gapped $\alpha - T_3$ lattices, *Phys. Rev. B* **103**, 165429 (2021).
- ⁴⁵ L. Mandhour and F. Bouhadida, Klein tunneling in deformed $\alpha - T_3$ lattice, arXiv:2004.10144 (2020).
- ⁴⁶ E. Illes and E. J. Nicol, Klein tunneling in the $\alpha - T_3$ model, *Phys. Rev. B* **95**, 235432 (2017).
- ⁴⁷ S. Peotta and P. Törmä, Superfluidity in topologically non-trivial flat bands. *Nat. Commun.* **6**, 8944 (2015).
- ⁴⁸ Aleksii Julku, Sebastiano Peotta, Tuomas I. Vanhala, Dong-Hee Kim, and Päivi Törmä, Geometric Origin of Superfluidity in the Lieb-Lattice Flat Band, *Phys. Rev. Lett.* **117**, 045303 (2016).
- ⁴⁹ J. Y. Vaishnav and Charles W. Clark, Observing Zitterbewegung with Ultracold Atoms, *Phys. Rev. Lett.* **100**, 153002 (2008)
- ⁵⁰ Bashab Dey and Tarun Kanti Ghosh, Floquet topological phase transition in the $\alpha - T_3$ lattice, *Phys. Rev. B* **99**, 205429 (2019)
- ⁵¹ Fa Wang and Ying Ran, Nearly flat band with Chern number $C = 2$ on the dice lattice, *Phys. Rev. B* **84**, 241103(R) (2011)
- ⁵² D. Bercioux, D.F. Urban, H. Grabert, and W. Häusler, Massless DiracWeyl fermions in a T_3 optical lattice. *Phys. Rev. A* **80** (6), 063603 (2009)
- ⁵³ D. D. Edwall, J. S. Chen, J. Bajaj, and E. R. Gertner, MOCVD Hg_{1-x}CdxTe/GaAs for IR detectors. *Semi cond. Sci. Technol.* **5**(3S), S221 (1990)
- ⁵⁴ Y. Betancur-Ocampo and V. Gupta, Perfect transmission of 3D massive Kane fermions in HgCdTe Veselago lenses. *J. Phys.: Condens. Matter.* **30**(3), 035501 (2017)
- ⁵⁵ R. Shen, L. B. Shao, B. Wang, and D. Y. Xing, Single Dirac cone with a flat band touching on line-centered-square optical lattices, *Phys. Rev. B* **81**, 041410(R) (2010).
- ⁵⁶ C. Xu, G. Wang, Z. Hang, J. Luo, C.T. Chan, and Y. Lai, Design of full-k-space flat bands in photonic crystals beyond the tight-binding picture, *Sci. Rep.* **5**, 18181 (2015).
- ⁵⁷ Seungchul Kim, Jisoon Ihm, Hyoung Joon Choi, and Young-Woo Son, Origin of Anomalous Electronic Structures of Epitaxial Graphene on Silicon Carbide, *Phys. Rev. Lett.* **100**, 176802 (2008).
- ⁵⁸ M.S. Nevius, M. Conrad, F. Wang, A. Celis, M.N. Nair, A. Taleb-Ibrahimi, A. Tejada, and E.H. Conrad, Semiconducting Graphene from Highly Ordered Substrate Interactions, *Phys. Rev. Lett.* **115**, 136802 (2015).
- ⁵⁹ S. Y. Zhou, G.-H. Gweon, A. V. Fedorov, P. N. First, W. A. de Heer, D.-H. Lee, F. Guinea, A. H. Castro Neto, and A. Lanzara, Substrate-induced bandgap opening in epitaxial graphene, *Nature Mater* **6**, 770 (2007).
- ⁶⁰ J. Romhányi, K. Penc, and R. Ganesh, Hall effect of triplons in a dimerized quantum magnet, *Nat. Commun.* **6**, 6805 (2015).
- ⁶¹ E. V. Gorbar, V. P. Gusynin, and D. O. Oriekhov, Electron states for gapped pseudospin-1 fermions in the field of a charged impurity, *Phys. Rev. B* **99**, 155124 (2019).
- ⁶² Dmitry Green, Luiz Santos, and Claudio Chamon, Isolated flat bands and spin-1 conical bands in two-dimensional lattices, *Phys. Rev. B* **82**, 075104 (2010).
- ⁶³ C. H. Yang, R. Wieser, and L. Wang, The effect of a variable coupling parameter on the tunneling properties from graphene to $\alpha - T_3$ model, *Journal of Applied Physics* **128**(9), 094301 (2020).