Competition of trivial and topological phases in patterned graphene based heterostructures

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We explore the impact of mechanical strain on the competition of topological and trivial gap generation mechanisms in patterned graphene based heterostructures. We focus on Kekulé-O type distortion favoring a trivial phase and commensurate Kane-Mele type spin-orbit coupling germinating a topological phase. We derive a simple low-energy Dirac Hamiltonian incorporating the two gap promoting effects and include terms corresponding to uniaxial strain. The derived effective model explains previous ab initio results elucidating a simple physical picture. We show that while the trivial gap is sensitive to mechanical distortions the topological gap stays resilient.

I. INTRODUCTION

Kekulé type patterned bond texture has potentially a dramatic impact on the electronic spectrum of graphene [1–3]. Specifically Kekulé-O type distortion, depicted in Fig. 1 scatters carriers between the two momentum space valleys of graphene resulting in the appearance of a band gap [3]. Andrade and coworkers have recently studied the effect of mechanical strain on the spectrum of Kekulé patterned samples [4]. They showed that strain substantially influences the gap generated due to a Kekulé-O pattern. As strain increases the gap closes pushing the sample from an insulator to a semimetal. Crucially these previous studies did not consider other gap generation mechanisms which may arise in samples compatible with Kekulé-O texture. In our previous work we show that in graphene based heterostructures, utilizing ternary bismuth tellurohalides, Kekulé distortion is accompanied by strong induced spin-orbit coupling [5, 6]. In these structures a competition between two gap generation mechanisms ensue. On the one hand Kekulé-O texture favors a trivial band gap, while the induced spin-orbit interaction drives a topological Kane-Mele type gap [7]. Consequently it has been found that mechanical distortions can drive the system from a trivial insulator to a topological phase.

In the present work, based on a simple tight-binding description we derive an analytical model explaining this phenomenon. Through an effective Dirac type Hamiltonian we show how the competition of the two type of gap promoting effects is tuned by mechanical distortions.
II. MODEL AND RESULTS

Let us consider the tight-binding model of a patterned graphene lattice as depicted in Fig. 1. Each first nearest neighbor bond carries a hopping amplitude of $t$. Kekulé-O distortion is taken into account through an additional $\Delta$ hopping term supplementing each bond around every third hexagon. These terms will be responsible for opening a trivial gap [3]. On the same hexagons the Kekulé-O distortion is active we also introduce a next nearest neighbour spin dependent hopping. For spin up electrons this corresponds to a hopping amplitude $im$ in the direction of the bond vectors denoted by arrows, while $-im$ for spin down particles. This term, adopted from the Kane-Mele model, promotes a topological gap [21]. Besides the considered bond texture discussed above we also incorporate a uniaxial in-plane strain in our description. We take into account the linear distortion of the lattice vectors and the exponential renormalization of all hopping terms. The topological flavor of the model can be obtained by determining the Wannier center flow [8, 9] of the tight-binding Hamiltonian defined above.

The following simplified low-energy Hamiltonian captures the most important electronic properties at the vicinity of the distorted Dirac-cones of graphene (for derivation of the model see the Appendix):

$$\hat{H} = v [\sigma A \otimes \tau_x \otimes s_0 + \sigma k \otimes \tau_x \otimes s_0] + \Delta \sigma_z \otimes \tau_x \otimes s_0 - m \cdot \sigma_z \otimes \tau_0 \otimes s_z,$$  \hspace{1cm} (1)

where $k$ is the momentum, $v = 3a_{cc}/2$ is the Fermi velocity (in units of $\hbar$) with $a_{cc} = 1.42 \text{Å}$ the equilibrium carbon-carbon bond distance [10]. The $\sigma = (\sigma_x, \sigma_y)$, $\tau_i$ and $s_i$ are the Pauli matrices. $\sigma_i$ are acting on the sub-lattice, $\tau_i$ on the valley degree of freedom while $s_i$ act on the real spin. The pseudovector potential $A$ describes mechanical distortions, specifically for the case of uniaxial in-plane strain its components are [11–14]:

$$A = \frac{\beta}{2a_{cc}} \varepsilon (1 + \rho) \left( \begin{array}{cc} \cos 2\theta \\ -\sin 2\theta \end{array} \right),$$ \hspace{1cm} (2)

where $\beta \approx 3$ is the Grüneisen parameter [15–17] that modulates the hopping terms of the tight-binding model as strain changes the intercarbon distance due to lattice deformations, $\varepsilon$ is the magnitude of the distortion, $\rho$ is the Poisson ratio, estimated to be $\rho \approx 0.165$ for graphene [18–20] while $\theta$ is the angular direction of the strain with respect to the $x$ axis.

Since Hamiltonian (1) is diagonal in the proper spin degree of freedom each spin species can be treated separately. Diagonalizing (1) yields the same spectrum for both spin orientations:

$$E (k) = \pm \sqrt{\xi^2 + \Delta^2 + v^2|k|^2 + m^2 \pm 2\sqrt{\xi^2 \Delta^2 + (v^2 A \cdot k)^2 + \Delta^2 m^2}},$$ \hspace{1cm} (3)

where we introduce

$$\xi = \frac{v \beta}{2a_{cc}} \varepsilon (1 + \rho).$$ \hspace{1cm} (4)

The low-energy spectrum of the considered tight-binding model [21] and the effective Dirac Hamiltonian [1] for various model parameters is shown in Fig. 2. In the first row we show a clean graphene sample under strain. As the magnitude of the mechanical distortion increases the two Dirac cones shift apart. In the second row a trivial gap opened by Kekulé pattern is closed by an ever increasing strain driving the system into a semimetallic phase. On the contrary, as it can be observed in the third row the topological gap opened by the Kane-Mele term is insensitive to the strength of distortion. In the last row both gap generation mechanism are active and $\Delta > m$ resulting in a trivial gap for the unstrained case. As strain is increased the gap is closed and reopened but now with a topological flavor.

Analysing the spectrum, depicted in Fig. 2, the conditions for sustaining a gap can be discerned. We find, that if the applied mechanical distortion is constrained as

$$\sqrt{2}\xi \leq \sqrt{\Delta^2 (\Delta^2 + 4m^2)} + \Delta^2,$$ \hspace{1cm} (5)

then the band extrema are at $k = (0, 0)$ and the magnitude of the gap is

$$E_G = 2\sqrt{\xi^2 + \Delta^2 + m^2} - 2\sqrt{\xi^2 \Delta^2 + \Delta^2 m^2}.$$ \hspace{1cm} (6)

The gap closes if $\xi = \sqrt{\Delta^2 - m^2}$ at which point valence and conduction band touch at a single point. If condition (5) is unsatisfied the band extrema are shifted to a finite momentum, the magnitude of the gap in this case is:

$$E_G = 2m \sqrt{1 - \frac{\Delta^2}{\xi^2}}.$$ \hspace{1cm} (7)

We note that the observations made above are insensitive to the direction of strain i.e. $\theta$, similarly to previous results [4–15].

The impact of strain on the competition between the two topologically distinct phases can be observed in
FIG. 2. The low-energy spectrum of the considered tight-binding model (A21), denoted by solid orange lines, and the effective Dirac Hamiltonian (1), depicted with dashed black lines, for various parameters. Topological gaps are indicated by blue opaque coloring, while trivial gaps are highlighted with red. In all panels $m = 0.04t$ and $\Delta = 0.08t$ unless indicated otherwise, for all cases $\theta = 0$.

FIG. 3. Here we plot the evolution of the magnitude and character of the gap as the function of the strength of the applied mechanical distortion based on (6) and (7). If only the Kekulé term is active, shown with solid lines, than the gap decreases linearly with increasing strain and once it is closed the system remains gapless. On the other hand if we only keep the next nearest spin-orbit coupling, indicated by dashed lines, the gap remains constant in the face of ever increasing strain. If $\Delta > m$, shown with dotted lines, the original trivial gap closes and a nontrivial gap opens as strain is increased. For $m > \Delta$, denoted by a dashdotted line, an initial smaller topological gap is increased by the application of mechanical distortions.

III. CONCLUSION

We studied the effects of uniaxial strain upon the electronic properties of a patterned graphene lattice hosting a Kekulé-O textured bond alternation and a commensurate Kane-Mele type spin-orbit coupling. Based on a tight-binding model we distilled an effective, low-energy Dirac Hamiltonian. Analyzing the spectrum of the model we explored the various gaped phases present in the sample. We found that while the trivial gap favored by the Kekulé-O distortion is destroyed by the strain, the topological gap generated by the considered spin-orbit term remains resilient. This observation can be understood from the following reasoning. The applied mechanical distortion moves the two Dirac cones of graphene from their initial position. The Kekulé term scatters particles between valleys, and hence it can only open a gap if the Dirac cones are aligned. The Kane-Mele term on the other hand does not mix valleys and the gap opened through it is insensitive to the position of the Dirac cones. These findings explain our previous ab initio results [5].

CONFLICTS OF INTEREST

There are no conflicts to declare.

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[1] O. Gamayun, V. Ostroukh, N. Gnezdilov, I. Adagideli, and C. Beenakker, Valley-momentum locking in a graphene superlattice with Y-shaped Kekulé bond texture, New Journal of Physics 20, 023016 (2018).

[2] C.-Y. Hou, C. Chamon, and C. Mudry, Electron fractionalization in two-dimensional graphene-like structures, Physical review letters 98, 186809 (2007).

[3] C. Chamon, Solitons in carbon nanotubes, Physical Review B 62, 2806 (2000).

[4] E. Andrade, R. Carrillo-Bastos, and G. G. Naumis, Valley engineering by strain in Kekulé-distorted graphene, Physical Review B 99, 035411 (2019).

[5] Z. Tajkov, D. Visontai, L. Oroszlány, and J. Koltai, Uniaxial strain induced topological phase transition in bismuth-telluride-graphene heterostructures, Nanoscale 11, 12704 (2019).

[6] Z. Tajkov, D. Visontai, L. Oroszlány, and J. Koltai, Topological phase diagram of bitex–graphene hybrid structures, Applied Sciences 9, 4330 (2019).

[7] C. L. Kane and E. J. Mele, Quantum spin hall effect in graphene, Phys. Rev. Lett. 95, 226801 (2005).

[8] R. Yu, X. L. Qi, A. Bernevig, Z. Fang, and X. Dai, Equivalent expression of z 2 topological invariant for band insulators using the non-abelian berry connection, Physical Review B 84, 075119 (2011).

[9] J. K. Asbóth, L. Oroszlány, and A. Pályi, A Short Course on Topological Insulators: Band Structure and Edge States in One and Two Dimensions 1st ed., Lecture Notes in Physics, Vol. 909 (Springer International Publishing, BerlinXXX, 2016).

[10] D. R. Cooper, B. D’Anjou, N. Ghattamaneni, B. Harack, M. Hilke, A. Horth, N. Majlis, M. Massicotte, L. Vandsburger, E. Whiteway, and V. Yu, Experimental Review of Graphene, ISRN Condens. Matter Phys. 2012, 1 (2012).

[11] H. Suzuura and T. Ando, Phonons and electron-phonon scattering in carbon nanotubes, Phys. Rev. B 65, 235412 (2002).

[12] J. L. Manes, Symmetry-based approach to electron-phonon interactions in graphene, Phys. Rev. B 76, 045430 (2007).

[13] F. Guinea, M. Katsnelson, and A. Geim, Energy gaps and a zero-field quantum hall effect in graphene by strain engineering, Nature Physics 6, 30 (2010).

[14] M. R. Masir, D. Moldovan, and F. Peeters, Pseudo magnetic field in strained graphene: Revisited, Solid State Communications 175, 76 (2013).

[15] G. G. Naumis, S. Barraza-Lopez, M. Oliva-Leyva, and H. Terrones, Electronic and optical properties of strained graphene and other strained 2d materials: a review, Reports on Progress in Physics 80, 096501 (2017).

[16] S. Reich, H. Jantoljak, and C. Thomsen, Shear strain in carbon nanotubes under hydrostatic pressure, Physical Review B 61, R13389 (2000).

[17] J. Gilvarry, Grüneneisen parameter for a solid under finite strain, Physical Review 102, 331 (1956).

[18] A. R. Botello-Mendez, J. C. Obeso-Jureidini, and G. G. Naumis, Toward an accurate tight-binding model of graphenes electronic properties under strain, The Journal of Physical Chemistry C 122, 15753 (2018).

[19] R. Faccio, P. A. Denis, H. Pardo, C. Goyenola, and A. W. Mombrú, Mechanical properties of graphene nanoribbons, Journal of Physics: Condensed Matter 21, 285304 (2009).

[20] F. Scarpa, S. Adhikari, and A. S. Phani, Effective elastic mechanical properties of single layer graphene sheets, Nanotechnology 20, 065709 (2009).

[21] P. E. Turchi, A. Gonis, and L. Colombo, Tight-Binding Approach to Computational Materials Science, Symposium Held December 1-3, 1997, Boston, Massachusetts, USA. Volume 491, Tech. Rep. (MATERIALS RESEARCH SOCIETY WARRENDALE PA, 1998).

Appendix A

In this section we give a detailed derivation of the Eq. (1) Hamiltonian in a didactic manner. We are interested in the Kekulé-O distorted graphene lattice hosting next-nearest neighbor Kane-Mele type spin-orbit interaction in the
perturbed hexagons under the influence of uniform, planar strain. *Id est*, the strain is position independent. The displacement field of the atoms due to the deformation is given by: $u(r) = \varepsilon \cdot r$. The actual position of the atoms are $r' = r + u(r) = (I + \varepsilon) r$, where $I$ is the $2 \times 2$ identity matrix.

$\varepsilon = \varepsilon \left( \cos^2 \theta - \rho \sin^2 \theta \right)$, \hspace{1cm} (A1)

where $\varepsilon$ is the magnitude of the applied strain, its angular direction, with respect to the $x$ axis, is $\theta$, and $\rho$ is the Poisson ratio, which relates the strain components (estimated to be $\rho = 0.165$ for graphene).

Our model consists of a tight-binding description of one $\pi$ orbital on every carbon site. We applied the above outlined formalism to include strain in our model, which can be formulated as:

$\hat{H} = \hat{H}_{Gr} + \hat{H}_{Kek} + \hat{H}_{SOI}$, \hspace{1cm} (A3)

where $\hat{H}_{Gr}$ describes the pristine graphene, $\hat{H}_{Kek}$ the Hamiltonian of the Kekulé-distortion and $\hat{H}_{SOI}$ the Hamiltonian of the Kane-Mele type model.

First let us consider the clean, pristine graphene. The structure of graphene is defined by a unit cell consisting of two equivalent atoms A and B. The lattice is spanned by the lattice vectors: $a_{21} = a_{cc} \frac{1}{2} (\pm \sqrt{3}, 3)$, where $a_{cc} \approx 1.42$ Å is the unperturbed carbon-carbon distance in the lattice. We define single particle states situated on sublattice $\alpha$:

$|\alpha, m \cdot a\rangle = |\alpha\rangle |m \cdot a\rangle$ and $|A\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, $|B\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$. \hspace{1cm} (A4)

where $m \cdot a$ runs over the atomic positions as $m \cdot a = m_1 a_1 + m_2 a_2$ over the pairs of integers. With this notation the tight-binding Hamiltonian for strained graphene in real space is given by:

$\hat{H}_{Gr} = \frac{t}{\sqrt{3}} \sum_{m} d_1 |B, m \cdot a \rangle \langle A, m \cdot a| + d_2 |B, m \cdot a \rangle \langle A, m \cdot a + a_1| + d_3 |B, m \cdot a \rangle \langle A, m \cdot a + a_2| + h.c.$, \hspace{1cm} (A5)
where \( t \approx 2.7 \text{ eV} \) is the hopping parameter for unstrained graphene. Introducing strain the hopping integrals depend on the direction of the bond due to the effect of strain, which can be taken into account with the following factors \cite{21, 23}:

\[
d_i = e^{-\beta \left( \frac{|v_{cc} \cdot \delta|}{a_{cc}} \right)} , \quad i = 1, 2, 3 , \tag{A6}
\]

where \( \beta \) is the Grüneisen parameter, estimated to be \( \beta \approx 3 \) for graphene and \( \delta_i \) are the bonding vectors pointing to one of the three nearest-neighbor sites at a given \( r \), as shown in Fig. 4\[\delta_1 = a_{cc} \left( 0, -1 \right), \delta_2 = a_{cc} / 2 \left( \sqrt{3}, 1 \right), \delta_3 = a_{cc} / 2 \left( -\sqrt{3}, 1 \right) .\]

Next let us consider the Kekulé-O distortion. The texture of the ordering is visualized in Fig. 4. The periodicity of the pattern differs from the pristine graphene and can be written as: \( A_1 = 2a_1 - a_2 \) and \( A_2 = -a_1 + 2a_2 \). We can formulate the Hamiltonian of the Kekulé-O texture in real space as:

\[
\hat{H}_{\text{Ko}} = \Delta \sum_M d_2 | B, M \cdot A \rangle \langle A, M \cdot A + a_2 | + d_3 | B, M \cdot A \rangle \langle A, M \cdot A + a_1 |
\]

\[
+ d_1 | B, M \cdot A + a_1 \rangle \langle A, M \cdot A + a_1 | + d_1 | B, M \cdot A + a_2 | \langle A, M \cdot A + a_2 |
\]

\[
+ d_2 | B, M \cdot A + a_2 \rangle \langle A, M \cdot A + a_2 | + d_3 | B, M \cdot A + a_1 | \langle A, M \cdot A + a_1 | + \text{h.c.},
\tag{A7}
\]

where \( M \) goes over the pairs integer numbers and \( \Delta \) is the strength of the distortion. (We note that our definition of \( \Delta \) is different from \cite{3}.)

The next part of our model is next-nearest-neighbor spin-orbit interaction. In order to preserve time-reversal symmetry we write the SOI term as \( \frac{im}{\sqrt{3}} \), where \( m \) is the strength of the interaction and has a positive value. We introduced an extra \( 1/\sqrt{3} \) factor in the magnitude of the interaction, which will be convenient later. The periodicity of the distortion is the same as in the case of the Kekulé term:

\[
\hat{H}_{\text{SOI}} = \frac{im}{\sqrt{3}} \sum_M d_4 | B, M \cdot A \rangle \langle B, M \cdot A + a_1 | + d_5 | B, M \cdot A + a_2 | \langle B, M \cdot A + a_2 |
\]

\[
+ d_5 | B, M \cdot A + a_1 \rangle \langle B, M \cdot A + a_1 | + d_5 | A, M \cdot A + a_1 | \langle A, M \cdot A + a_1 |
\]

\[
+ d_4 | A, M \cdot A + a_1 + a_2 \rangle \langle A, M \cdot A + a_2 | + d_6 | A, M \cdot A + a_2 | \langle A, M \cdot A + a_2 | + \text{h.c.}.
\tag{A8}
\]

The factors \( d_4, 5, 6 \) of the hopping integrals have a different form due to the different bonding vectors:

\[
d_4 = e^{-\beta \left( \frac{|v_{cc} \cdot \delta_1|}{a_{cc}} \right)} , \quad d_5 = e^{-\beta \left( \frac{|v_{cc} \cdot \delta_2|}{a_{cc}} \right)} , \quad d_6 = e^{-\beta \left( \frac{|v_{cc} \cdot (\delta_1 - \delta_2)|}{a_{cc}} \right)}. \tag{A9}
\]

In order to get the dispersion relation we must take the Fourier transform of our Hamiltonian \( \text{[A2]} \). We define the transformation via the following relations \cite{24}:

\[
| B, m \cdot a \rangle = \frac{1}{\sqrt{N}} \sum_k e^{ikm} a | B, k \rangle , \tag{A10}
\]

\[
| A, m \cdot a \rangle = \frac{1}{\sqrt{N}} \sum_k e^{ik(m \cdot a + \delta_1)} | A, k \rangle ,
\]

where \( N \) is the number of the unit cells.

While calculating the Hamiltonian in \( k \)-space is in principle straightforward, we impart a couple of remarks. Using the definition in Eq. \( \text{[A10]} \) we perform the Fourier transformation of the first term in Eq. \( \text{[A5]} \):

\[
\sum_m d_1 | B, m \cdot a \rangle \langle A, m \cdot a | = \frac{d_1}{N} \sum_m \sum_{k', k} e^{ikm} e^{-ik'} a e^{-ik' (m \cdot a + \delta_1)} | B, k \rangle | A, k' \rangle \tag{A11}
\]

\[
= \frac{d_1}{N} \sum_m \sum_{k', k} e^{im (a (k - k') + \delta_1)} e^{-ik' \delta_1} | B, k \rangle | A, k' \rangle .
\]
Examine more closely the following term:

\[ \sum_{m} e^{im \cdot a(k-k')} = \sum_{m_{1}=1}^{N_{1}} \sum_{m_{2}=1}^{N_{2}} e^{i(m_{1}a_{1}+m_{2}a_{2})\Delta k}, \tag{A12} \]

where \( N_{1} \cdot N_{2} = N \) and \( \Delta k = k - k' \). Write the \( \Delta k \) term as a linear combination of the reciprocal lattice vectors: \( \Delta k = \Delta k_{1} \cdot b_{1} + \Delta k_{2} \cdot b_{2} \), where \( \Delta k_{i} = \frac{2\pi}{N} \), with \( n = 0...N_{i} - 1 \). Plugging this back to Eq. (A12):

\[ \sum_{m} e^{im \cdot a(k-k')} = \sum_{m_{1}=1}^{N_{1}} e^{2\pi i m_{1} \Delta k_{1}} \sum_{m_{2}=1}^{N_{2}} e^{2\pi i m_{2} \Delta k_{2}} = N_{1}\delta_{\Delta k_{1},0} \cdot N_{2}\delta_{\Delta k_{2},0}, \tag{A13} \]

where \( \delta_{i,j} \) is the Kronecker symbol \([25, 26]\). Applying this to Eq. (A11) we get that

\[ \sum_{m} d_{1} |B, m \cdot a \rangle \langle A, m \cdot a| = d_{1} \sum_{k} e^{-ik\delta_{1}} |B, k \rangle \langle A, k|. \tag{A14} \]

The Fourier transformation of the terms with different periodicity must be done in the same manner. We show the first term of Eq. (A7) as an example:

\[ \sum_{M_{1},M_{2}} |B, M_{1} A_{1} + M_{2} A_{2} \rangle \langle A, M_{1} A_{1} + M_{2} A_{2} + a_{2}| \tag{A15} \]

\[ = \frac{1}{N} \sum_{k,k'} \sum_{M_{1},M_{2}} e^{ik(M_{1}(2a_{1} - a_{2}) + M_{2}(2a_{2} - a_{1}))} |B, k \rangle e^{-ik'(M_{1}(a_{1} - 2a_{2}) + M_{2}(2a_{2} - a_{1}) + a_{2})} e^{-ik'\delta_{1}} |A, k'| \]

\[ = \frac{1}{N} \sum_{k,k'} \sum_{M_{1},M_{2}} |B, k \rangle \langle A, k'| e^{-i(k'-k)(M_{1}(a_{1} - 2a_{2}) + M_{2}(2a_{2} - a_{1}))} e^{-ik'(a_{2} + \delta_{1})}. \]

Summing the terms that depend on \( M_{i} \), we get:

\[ \sum_{M_{1}=1}^{N_{1}} \sum_{M_{2}=1}^{N_{2}} e^{-i(k'-k)(M_{1}(2a_{1} - a_{2}) + M_{2}(2a_{2} - a_{1}))} \tag{A16} \]

where \( N_{1} \cdot N_{2} = N/3 \). We can rewrite the terms in the exponent as:

\[ M_{1}(2a_{1} - a_{2}) + M_{2}(2a_{2} - a_{1}) = (a_{1} \quad a_{2}) \begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix} \begin{pmatrix} M_{1} \\ M_{2} \end{pmatrix}. \tag{A17} \]

We can do the same expansion in the terms of the reciprocal lattice vectors as we did above:

\[ (\Delta k_{1} \quad \Delta k_{2}) \begin{pmatrix} b_{1} \\ b_{2} \end{pmatrix} \begin{pmatrix} a_{1} \quad a_{2} \\ 2 & -1 \\ -1 & 2 \end{pmatrix} \begin{pmatrix} M_{1} \\ M_{2} \end{pmatrix} = 2\pi (\Delta k_{1} \quad \Delta k_{2}) \begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix} \begin{pmatrix} M_{1} \\ M_{2} \end{pmatrix}. \tag{A18} \]

If this exponent is an integer number then the value of the expression is 1 and 0 otherwise. Which means we can translate the question to a set of linear equations and solve it over the integer numbers keeping in mind the fact that the \( \Delta k_{i} \) numbers have a finite set. This problem has 3 different solutions: \( k - k' = 0, \pm G \), where \( G = \frac{1}{3}(b_{1} - b_{2}) \) is the so-called Kekulé wave vector \([11, 27]\):

\[ \sum_{M_{1}=1}^{N_{1}} \sum_{M_{2}=1}^{N_{2}} e^{-i(k'-k)(M_{1}(a_{1} - 2a_{2}) + M_{2}(2a_{2} - a_{1}))} = \frac{N}{3} (\delta_{k,k'} + \delta_{k,k'+G}). \tag{A19} \]

Now we can write down the Fourier transform:

\[ \sum_{M_{1},M_{2}} |B, M_{1} A_{1} + M_{2} A_{2} \rangle \langle A, M_{1} A_{1} + M_{2} A_{2} + a_{2}| = \]

\[ \frac{1}{3} \sum_{k} |B, k \rangle \langle A, k| e^{-ik\delta_{1}} + |B, k \rangle \langle A, k + G| e^{-i(k + G)\delta_{2}} + |B, k \rangle \langle A, k + G| e^{-i(k - G)\delta_{2}}. \tag{A20} \]
Transforming every term in the Eq. [A26] Hamiltonian $\hat{h}$ becomes:

$$\hat{h}(k) = \Psi_k \left( \begin{array}{c} \Omega \\ \Gamma \end{array} \right) \left( \begin{array}{c} \Gamma^* \\ -\Omega^* \end{array} \right) \Psi_k^\dagger,$$

(A21)

where

$$\Psi_k = \left( \begin{array}{c} |Bk\rangle |B, k + G\rangle |B, k - G\rangle |A, k\rangle |A, k + G\rangle |A, k - G\rangle \end{array} \right),$$

(A22)

$$\Gamma = \left( \begin{array}{ccc} \left( t + \frac{2\Delta}{3} \right)s(k, 0)/2 & \frac{\Delta}{3}s(k, G) & \frac{\Delta}{3}s(k, -G) \\
\frac{\Delta}{3}s(k + G, -G) & \left( t + \frac{2\Delta}{3} \right)s(k + G, 0)/2 & \frac{\Delta}{3}s(k + G, G) \\
\frac{\Delta}{3}s(k - G, G) & \frac{\Delta}{3}s(k - G, -G) & \left( t + \frac{2\Delta}{3} \right)s(k - G, 0)/2 \end{array} \right),$$

(A23)

$$\Omega = \frac{im}{3\sqrt{3}} \left( \begin{array}{ccc} s'(k, 0) - s^*(k, 0) & s'(k, G) - s^*(k, G) & s'(k, -G) - s^*(k, -G) \\
s'(k + G, 0) & s'(k + G, -G) & s'(k + G, 0) \\
s'(k - G, 0) & s'(k - G, -G) & s'(k - G, 0) \end{array} \right).$$

(A24)

We introduced the following functions:

$$s(k, p) = d_1 e^{-ik(1+\epsilon)\delta_1} (e^{-ip\delta_1} + e^{-ip\delta_2}) + d_2 e^{-ik(1+\epsilon)\delta_2} (e^{ip\delta_1} + e^{-ip\delta_2}) + d_3 e^{-ik(1+\epsilon)\delta_3} (e^{-ip\delta_3} + e^{ip\delta_1})$$

$$s'(k, p) = d_4 e^{-ik(1+\epsilon)\alpha_1} e^{-ip\alpha_1} + d_5 e^{ik(1+\epsilon)\alpha_2} e^{ip\alpha_2} + d_6 e^{-ik(1+\epsilon)\alpha_2} e^{-ip\alpha_2}.$$  

(A25)

(A26)

In order to obtain the desired low-energy approximation of the [A21] Hamiltonian we neglect the terms that correspond to the high energy bands. As a result we redefine the vector of states following the convention of Andrade et. al [4] as:

$$\Psi_k = \left( \begin{array}{c} -|A, k - G\rangle |B, k - G\rangle |B, k + G\rangle |A, k + G\rangle \end{array} \right).$$

(A27)

Strain alters the hopping energies as it was introduced in Eq. [A6]. We expand the corresponding factors up to the first order in strain:

$$d_i \approx 1 - \beta \left( \frac{\langle \epsilon + I \rangle \delta_i}{a_{cc}} - 1 \right) = 1 - \beta \left( \frac{\sqrt{\epsilon \delta_i + \delta_i^*} (\epsilon \delta_i + \delta_i)}{a_{cc}} - 1 \right) \approx 1 - \beta \frac{\delta_i^* \epsilon \delta_i}{a_{cc}^2}.$$

(A28)

Next we proceed to expand [A21] up to first order in $k$. To this end we can make an expansion of the energy dispersion relations $s$ and $s'$ around $G$. However, as other works already have shown, it is necessary to expand around the true Dirac points, which are defined as the zeros of the deformed lattice energy dispersion. Generally these are located neither at the high-symmetry points of the strained lattice nor at the original Dirac cones’s tips. These new $k$-points are given by $K = \pm (G + A)$. [14] [15] [18] [28]

Expanding the [A21] Hamiltonian with the above written formalism results in the following effective Hamiltonian:

$$\hat{H}_{\text{eff}}(k) = -\frac{3}{2} \left( t + \frac{2\Delta}{3} \right) |\sigma A \otimes \tau_+ + |\sigma (1 + (1 - \beta) \epsilon) k \otimes \tau_0| - \frac{\Delta}{2} \left[ (\beta \epsilon p \epsilon - 2) \sigma_2 \otimes \tau_x + (A \times k)_x \sigma_0 \otimes \tau_y + Ak \sigma_0 \otimes \tau_x + \right.$$

$$\left. m \left[ Ak \sigma_2 \otimes \tau_x - \left( \frac{1}{2} \beta \epsilon p (\epsilon - 1) \sigma_2 \otimes \tau_0 \right) - m \left( (Mk)_x - i(Mk)_y, (M^*k)_x + i(M^*k)_y \right) + [(I + \epsilon) k] \sigma \right] \otimes \tau_x, \right.$$

(A29)

where $M = aI \epsilon p (\epsilon - 2) \sigma_2 \otimes \tau_x$ with $4a = -1 + \sqrt{3}i$ and $2b = -1 - \sqrt{3}i$.

We can simplify this formula further by focusing on the case when the perturbation in $m$ and $\Delta$ also can be considered small. With this simplification and plugging back the spin degree of freedom we get:

$$\hat{H}_{\text{low-energy}} = v \left[ |\sigma A \otimes \tau_+ + |\sigma k \otimes \tau_0| \otimes \sigma_0 + \Delta \cdot \sigma_2 \otimes \tau_x \otimes \sigma_0 - m \cdot \sigma_2 \otimes \tau_0 \otimes \sigma_2, \right.$$

(A30)

which is equivalent to our simplified low-energy Hamiltonian in Section [II] at Eq. (1), where, for convenience, we omitted the ‘low – energy’ label.