Valley engineering by strain in Kekulé-distorted graphene

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A Kekulé bond texture in graphene modifies the electronic band structure by folding the Brillouin zone and bringing the two inequivalent Dirac points to the center. This can result, in the opening of a gap (Kek-O) or the locking of the valley degree of freedom with the direction of motion (Kek-Y). We analyze the effects of uniaxial strain on the band structure of Kekulé-distorted graphene for both textures. Using a tight-binding approach, we introduce strain by considering the hopping renormalization and corresponding geometrical modifications of the Brillouin zone. We numerically evaluate the dispersion relation and present analytical expressions for the low-energy limit. Our results indicate the emergence of a Zeeman-like term due to the coupling of the pseudospin with the pseudomagnetic strain potential which separates the valleys by moving them in opposite directions away from the center of the Brillouin zone. For the Kek-O phase, this results in a competition between the Kekulé parameter that opens a gap and the magnitude of strain which closes it. While for the Kek-Y phase, in a superposition of two shifted Dirac cones. As the Dirac cones are much closer in the superlattice reciprocal space that in pristine graphene, we propose strain as a control parameter for intervalley scattering.

I. INTRODUCTION

In graphene, the electronic properties are dominated by the two inequivalent local minima in the conduction band, located at the high symmetry Brillouin zone points \( K_+ \) and \( K_- \), and referred to the \( K_D^+ \) and \( K_D^- \) valley, respectively. This endows low-energy electrons with an additional degree of freedom, known as valley isospin. In pristine membranes, these two valleys have gapless Dirac spectra, which are degenerate in energy, related by time-reversal symmetry, and well separated in reciprocal space by the Kekulé vector \( G = K_+ - K_- \). However, if graphene is subject to a periodic perturbation, with a spatial periodicity associated with \( G \) (Kekulé distortion), a superlattice with a tripled unit cell (of the size of a hexagonal ring) is formed. As a consequence, the two Dirac cones at opposite corners \( (K_D^+ \text{ and } K_D^-) \) are folded onto the center \( \Gamma \) of the new hexagonal superlattice Brillouin zone. Almost twenty years ago, Claudio Chamon showed that a bond distortion mimicking the Kekulé structure for benzene (Kek-O) provides such a periodicity in graphene, which opens a gap by mixing the two valley species. Interestingly, graphene with a Kek-O distortion is also expected to show topological charge fractionalization, and other topological properties.

Although experimentally achievable in analogues of graphene, up to now the Kek-O phase in graphene has not become a physical reality. Nevertheless, theoretical studies suggest that the Kek-O phase can be obtained by depositing graphene on top of a topological insulator, by applying uniaxial strain or by placing atoms adsorbed on its surface. The latter proposal was pursued by Gutierrez et al., who experimentally found another Kekulé distortion, the Kekulé-Y (Kek-Y) phase, which consists of a periodic modification of the three bonds (in form of the letter Y) surrounding one of the atoms of the new hexagonal unit cell. Recently, Gamayun et al. showed that this Kek-Y bond texture results in the locking of valley isospin with the direction of motion (momentum), breaking the valley degeneracy while preserving the massless character of the Dirac fermions. This effect opens a new way to control the valley degree of freedom in graphene.

There have been several theoretical proposals to manipulate the valley degree of freedom in graphene, including the celebrated Valley Hall effect produced by Berry curvature, and the use of strain. The former has been recently observed in graphene superlattices by nonlocal transport measurement. The effects of the latter are strong, measurable and expected to be valley asymmetric. In fact, both couple asymmetrically with each valley by breaking the inversion symmetry while preserving time reversal. Nevertheless, strain offers the advantage of being tunable and it is in intimate relation with the Kekulé phase, since this phase is expected to appear in the presence of uniaxial strain. In general, uniaxial strain alters the band structure of graphene by (1) distorting the shape of the Brillouin zone, thus changing the geometrical position of the high symmetry points due to the modification of the lattice vectors, and (2) moving the Dirac cones away from the high symmetry points, since it changes unevenly the three hopping energies connecting neighboring sites. These two effects should be taken into account to obtain the low energy approximation for graphene, otherwise unphysical results are obtained even in the simplest cases.

Inspired by the results described above, in the present manuscript we evaluate the effect of uniaxial strain on Kekulé distorted graphene in both phases: Kek-O and Kek-Y. Using the tight binding approximation, we write...
Given that graphene, $\Delta = \epsilon \delta$ and $r_{\text{sublattice B}}$, and surrounding the site located at a given amplitude $\Delta$ describing the bond-density wave of the Kekulé pattern such that the Kekulé wave vector is $G$ such that the Kekulé wave vector is $G$.

Let us now consider the effects of strain. When a strain field $u = (u_x(x,y), u_y(x,y))$ is applied to pristine graphene, the atomic positions $r$ change to,

$$r' = (1 + \tilde{\epsilon}) \cdot r,$$

where $\tilde{\epsilon}$ is the strain tensor with components,

$$\epsilon_{ij} = \frac{1}{2} \left( \frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right).$$

The lattice vectors are $a = a(-\sqrt{3}/2, \frac{3}{2})$, and $a = a(\sqrt{3}/2, \frac{3}{2})$, with $a = 1.42$ Å. Each vector $\delta_i$ points to one of the three nearest-neighbor sites belonging to sublattice B, and surrounding the site located at a given $r$, as shown in Fig. 1 $[\delta_1 = a(\sqrt{3}/2, -\frac{1}{2}), \delta_2 = -a(\sqrt{3}/2, \frac{1}{2})$, and $\delta_3 = a(0,1)]$. The set of tight-binding parameters describing the bond-density wave of the Kekulé pattern is given by

$$t_{r,j} = t_0 \left[ 1 + \Delta e^{i(pK_+ + qK_-) \delta_j + iG \cdot r} + \Delta^* e^{-i(pK_+ + qK_-) \delta_j - iG \cdot r} \right],$$

where $t_0 \approx 2.7 eV$ is the hopping-parameter for pristine graphene, $\Delta = e^{i2\pi m/3} \Delta_0$ is the Kekulé coupling with amplitude $\Delta_0$ and $m$ an arbitrary integer number, $K_\pm = \frac{2\pi}{\sqrt{3}} \sqrt{3}(\pm 1, \pm 3)$ are the high-symmetry points of graphene such that the Kekulé wave vector is $G = \frac{4\pi}{3\sqrt{3}}(1,0)$. Given that $p$ and $q$ are integers, the value of the Kekulé-distorted hopping-parameter $t_{r,j}$ oscillates in space between the values $t_0(1 - \Delta_0)$ and $t_0(1 + 2\Delta_0)$, generating a Kekulé texture accordingly to the index

$$\nu = 1 + q - p \mod 3,$$

with a Kek-O texture for $\nu = 0$, and Kek-Y for $\nu = \pm 1$.

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where $i = x, y$ and $j = x, y$. The local distance between neighbor atoms gets modified accordingly,

$$\delta_j' = (1 + \tilde{\epsilon}) \cdot \delta_j,$$

and similarly the basis vectors,

$$a_j' = (1 + \tilde{\epsilon}) \cdot a_j,$$

as seen in Fig. 1.

Notice that the considered strain is uniform and thus space independent. This case also serves as a first approximation for smooth strain profiles. As the strain is uniform, it can be written as follows,

$$\tilde{\epsilon} = \begin{bmatrix} \epsilon_{xx} & \epsilon_{xy} \\ \epsilon_{yx} & \epsilon_{yy} \end{bmatrix} = \begin{bmatrix} \epsilon_Z & \epsilon_S \\ \epsilon_S & \epsilon_A \end{bmatrix}.$$

II. HAMILTONIAN FOR STRAINED KEKULÉ DISTORTED GRAPHENE

Let us start by considering a pure Kekulé pattern on unstrained graphene. The electronic properties are well described by a tight-binding Hamiltonian for a single $\pi$-orbital per carbon site,

$$H = -\sum_r \sum_{j=1}^3 t_{r,j} a_r^\dagger b_{r+\delta_j} + H.c.,$$

where $r$ runs over the atomic positions of graphene’s sub-lattice $A$, given by $r = n_1 a_1 + n_2 a_2$, with $n_1$ and $n_2$ integers. The lattice vectors are $a_1 = a(-\frac{\sqrt{3}}{2}, \frac{3}{2})$, and $a_2 = a(\frac{\sqrt{3}}{2}, \frac{3}{2})$, with $a = 1.42$ Å. Each vector $\delta_i$ points to one of the three nearest-neighbor sites belonging to sublattice B, and surrounding the site located at a given $r$, as shown in Fig. 1 $[\delta_1 = a(\frac{\sqrt{3}}{2}, -\frac{1}{2}), \delta_2 = -a(\frac{\sqrt{3}}{2}, \frac{1}{2})$, and $\delta_3 = a(0,1)]$. The set of tight-binding parameters describing the bond-density wave of the Kekulé pattern is given by

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where $t_0 \approx 2.7 eV$ is the hopping-parameter for pristine graphene, $\Delta = e^{i2\pi m/3} \Delta_0$ is the Kekulé coupling with amplitude $\Delta_0$ and $m$ an arbitrary integer number, $K_\pm = \frac{2\pi}{\sqrt{3}} \sqrt{3}(\pm 1, \pm 3)$ are the high-symmetry points of graphene such that the Kekulé wave vector is $G = \frac{4\pi}{3\sqrt{3}}(1,0)$. Given that $p$ and $q$ are integers, the value of the Kekulé-distorted hopping-parameter $t_{r,j}$ oscillates in space between the values $t_0(1 - \Delta_0)$ and $t_0(1 + 2\Delta_0)$, generating a Kekulé texture accordingly to the index

$$\nu = 1 + q - p \mod 3,$$

with a Kek-O texture for $\nu = 0$, and Kek-Y for $\nu = \pm 1$.

FIG. 1. Lattices and Brillouin Zones for: (a) pristine graphene, (b) Kek-Y distorted graphene (red bonds), (c) strained graphene, and (d) Kek-Y distorted graphene with strain. The Kekulé and strained Kekulé vectors $G$ and $G'$ are indicated in the upper side of the hexagonal Brillouin zones for each case. In a), the Dirac cones for pristine graphene are indicated in dark gray. In b), the gray Dirac cones are folded into a degenerate Dirac cone (in blue) to the $\Gamma$ point, while in c), the original Dirac cones (in gray) are deformed and translated to the points $K_{D'}$ as indicated in red. In d), the Dirac cones (gray) are folded into the $\Gamma$ point, but the strain breaks the degeneracy resulting in the overlapping of two shifted Dirac cones, both indicated in purple.
In the previous expression, the space-independent parameters $\epsilon_s$ and $\epsilon_z$ denote uniaxial strain applied along the zigzag and armchair directions, respectively, and $\epsilon_s$ is the shear strain. This tensor can be parametrized in terms of $\epsilon$ (the magnitude of the applied strain), its angular direction $\theta$ (with respect to the $x$-axis), and $\rho$, the Poisson ratio which relates the strain components with a value of $\rho = 0.165$ for graphene\(^{31}\),

$$\bar{\epsilon} = \left[ \epsilon (\cos^2 \theta - \rho \sin^2 \theta) \epsilon (1 + \rho) \cos \theta \sin \theta \right].$$

(9)

In the absence of a Kekulé pattern, the tight-binding parameter for the strained lattice is given by\(^{40}\)

$$t_j = t_0 e^{-\beta \left( \frac{|\delta j|}{2} - 1 \right)},$$

(10)

where $\beta$ is the Gruneissen parameter, estimated to be $\beta \approx 3$ for graphene. It is important to remark that second- and third-neighbor interactions are always present, which depend upon the bond torsion-angle\(^{51}\). These effects will be neglected here as a first approximation.

Now, we can combine strain with a Kekulé pattern as follows: First, due to the modified distance between sites, the tight-binding parameter $t_0$ in Eq. (2) is replaced by $t_j$, defined by Eq. (10). Second, we need to keep the Kekulé density-wave bond ordering. Thus, we can proceed by observing that the phases of the pattern are preserved if\(^{43}\)

$$(pK_+ + qK_-) \cdot \delta j + G \cdot r = (pK'_+ + qK'_-) \cdot \delta j' + G' \cdot r',$$

(11)

as long as we define,

$$K'_+ = (1 + \epsilon)^{-1} \cdot K_+,$$

(12a)

$$G' = K'_+ - K'_- = (1 + \epsilon)^{-1} \cdot G.$$

(12b)

this constitutes a systematical procedure to introduce uniaxial strain to graphene superlattices.

Although it is tempting to think of $K'_+$ as the reciprocal transformation of Eq. (4) for the high-symmetry points of the deformed lattice, in general, it turns out that the transformed reciprocal vectors of the high symmetry points of pristine graphene do not coincide with the high-symmetry points of the deformed lattice Brillouin zone\(^{40,49}\). Moreover, strain changes the symmetry of the Bravais lattice. The high-symmetry points of the first Brillouin zone strained lattice must be labeled differently. As an example, the $K_+$ points of the P6/mmm space group after a uniaxial strain are replaced by the $F_0$ and $\Delta_0$ points in the Cmmm space group\(^{40}\). Also, we stress out that Dirac points $K'_\pm$ corresponding to the deformed lattice energy dispersion do not necessarily coincide neither with $K'_\pm$ nor with $F_0$ or $\Delta_0$. Fig. 1 brings a sketch of these general observations, and serves as a warning to avoid confusions about such aspects\(^{40}\).

The modification of the tunneling parameter [Eq. (2)] and the change of the pattern phases [Eq. (11)] caused by strain result in a new set of tight-binding parameters $\tilde{t}_{\nu'j}$:

$$\tilde{t}_{\nu'j} = t_j \left[ 1 + \Delta \epsilon^{\pm}(pK'_+ + qK'_-) \cdot \delta j' + G' \cdot r' + \Delta \epsilon^{*} e^{\mp i(pK'_+ + qK'_-) \cdot \delta j' - iG' \cdot r'} \right].$$

(13)

Therefore the new Hamiltonian for the applied strain on a Kekulé pattern is the following,

$$H = -\sum_{\nu'} \sum_{j} \tilde{t}_{\nu'j} a_{\nu'j}^\dagger b_{\nu'j} + H.c.$$  

(14)

Such a Hamiltonian can be written in reciprocal space by taking a Fourier transform of the annihilation/creation operators. The three terms in Eq. (13) lead to Hamiltonian $H(k) = H_1(k) + H_2(k) + H_3(k)$, where $H_1(k)$ is the contribution from the Fourier transform that arises from Eq. (14) by considering the first term in Eq. (13):

$$H_1(k) = -\frac{1}{2\pi} \sum_{\nu',j} \int_{k,k''} t_{j} a_{\nu'k}^\dagger b_{\nu'k''} e^{i\nu' \cdot (k-k'')} d^2k d^2k'',$$

$$= -\int_{k} \sum_{\nu,j} t_{j} a_{\nu'k}^\dagger b_{\nu'k} e^{i\nu'j + i\epsilon k \cdot \delta j + iG' \cdot r'} d^2k,$$

$$= -\int_{k} s'(k) a_{\nu'k}^\dagger b_{\nu'k} d^2k,$$

(15)

where $s'(k)$ is the dispersion relation for strained graphene without the Kekulé pattern,

$$s'(k) = \sum_{\nu,j} t_{j} e^{i\epsilon k \cdot \delta j}.$$  

(16)

The second term, $H_2(k)$, is
$H_2(k) = -\frac{\Delta}{2\pi} \sum_{r',j} \int_{k_-,k_+} t_j a^\dagger_{k_0} b_k e^{i(K'_+ + qK'_-)} \delta'_j e^{-i\rho' \cdot (k'' - (k' + G'))} d^2k d^2k''$, 

$$= -\Delta \int_k s'(k + pK'_+ + qK'_-) a^\dagger_{k_g} b_k d^2k,$$

where, 

$$H(k) = -s'(k)a^\dagger_k b_k - \Delta s'(k + pK'_+ + qK'_-) a^\dagger_{k + G'} b_k$$

This expression can be rewritten in terms of a $6 \times 6$ matrix, by defining the column vector $c_k = (a_k, a_{k-G'}, a_{k+G'}, b_k, b_{k-G'}, b_{k+G'})$, resulting in,

$$H(k) = -c^\dagger_k \begin{pmatrix} 0 & \Gamma \end{pmatrix} c_k,$$

where,

$$\Gamma = \begin{pmatrix} s'(k) & \Delta s'(k - G' + pK'_+ + qK'_-) & \Delta^* s'(k + G' - pK'_+ - qK'_-) \\
\Delta^* s'(k - G') & s'(k + G' - pK'_+ - qK'_-) & \Delta s'(k + G' + pK'_+ + qK'_-)
\end{pmatrix}.$$

Eq. (20) can be further simplified by using the relation

$$s'(k + pK'_+ + qK'_-) = e^{i\frac{2\pi}{p+q}} s'(k + (\nu - 1)G')$$

and defining $\tilde{\Delta} = e^{i\frac{2\pi}{p+q}} \Delta$ and $s'_n = s'(k + nG')$, to obtain,

$$\Gamma = \begin{pmatrix} s'_0 & \tilde{\Delta}s'_{\nu+1} & \tilde{\Delta}^* s'_{-\nu-1} \\
\tilde{\Delta}^* s'_{-\nu} & s'_1 & \tilde{\Delta}s'_{-\nu-1}
\end{pmatrix}.$$

As a result, the spectrum is symmetric around $E = 0$ and is determined by $|\Gamma|^2 = \Gamma^\dagger \Gamma$. To illustrate this, we simply calculate

$$H^2(k) = -c^\dagger_k \begin{pmatrix} |\Gamma|^2 & 0 \\
0 & |\Gamma|^2
\end{pmatrix} c_k,$$

with characteristic polynomial,

$$\det \left( |\Gamma|^2 - E^2(k) \right) = 0.$$

In Figure 2 we show a comparison between the energy dispersions for (a) graphene with a Kek-O pattern, (b) graphene with a Kek-Y pattern, (c) with a Kek-O pattern and strain, and (d) with a Kek-Y pattern and strain. From Fig. 2(a) and Fig. 2(c) it is clear that a gap is preserved for small values of $\epsilon$, although its size is considerable reduced when compared with the pure Kek-O pattern. This results from a competition between the Kekl parameter that opens a gap and the magnitude of strain which closes it. Once the gap is closed, an increase of the strain results in two shifted Dirac cones (not shown).

Figure 2 (d) shows the results for a Kek-Y pattern with strain. Here, the effects of strain are much more important, as the central Dirac cones are no longer uniaxial, resulting in two separate Dirac cones. For this phase, strain preserves the massless character and moves
the cones away from the center of the Brillouin zone. In Figure 1 we provide a short pictorial summary of the Dirac cones’ fate after applying a pure Kekulé, strain, or a Kekulé plus strain modulations. For the case of Kekulé plus strain, the tips of the two cones are much closer in reciprocal space than in the case of graphene. This suggests that strain can be used to control the distance between valleys to do valley engineering. As the electrical conductivity\(^{52}\) and the optical properties\(^{35,34}\) depend upon the distance in k-space of the cone tips, it is clear that strain valley engineering can be much more effective in Kekulé patterns than in pure graphene. In the following section, we will consider a low energy approximation that allows us to obtain a useful effective Dirac Hamiltonian for this system.

### III. LOW-ENERGY APPROXIMATION

In order to obtain an effective Hamiltonian for low energies, we start by observing that the first row and column of the matrix \(\Gamma\) given by Eq. (22) are negligible in such limit, since they correspond to the high energy bands depicted in brown and blue in Figure 2. As a result, we can redefine the column vector of annihilation operators as \(u_k = (a_{k-G'}, a_{k-G'}, b_{k-G'}, b_{k+G'})\). The effective Hamiltonian now can be written as follows,

\[
H_{\text{eff}} = -u_k^\dagger \begin{pmatrix} 0 & 0 & s'_{-1} & \tilde{s}'_{1} \\ 0 & 0 & \tilde{s}'_{s} & 0 \\ \tilde{s}'_{s} & 0 & 0 & 0 \\ \tilde{s}'_{s} & 0 & 0 & 0 \end{pmatrix} u_k.
\] (25)

Next, we proceed to expand Eq. 25 to first order in \(k\). To this end we can make an expansion of the energy dispersion \(s'_{s}\) around \(nG'\). However, as other works have shown\(^{40,48}\), it is necessary to expand around the true Dirac points, which are defined as the zeros of the deformed lattice energy dispersion, not located at the high-symmetry points of the strained-lattice, or at the original Dirac cones’ tips. These new Dirac points are given by \(K_D^{\pm} = (G' + A)\), where \(A\) is the pseudo-magnetic vector potential\(^{40,48}\), whose explicit form depends upon the components of the strain tensor \(\epsilon\):

\[
A_x = \frac{\beta}{2\alpha}(\epsilon_{xx} - \epsilon_{yy}), \quad A_y = -\frac{\beta}{2\alpha}(2\epsilon_{xy}).
\] (26)

By writing \(s'_{s}\) as \(s'((k + nG' + nA - nA) = s'((k - nA) + nK_D^{\pm})\) we can explicitly ensure that the expansion is performed around the true Dirac points. Then we return to \(nG'\) through a translation of \(-nA\), such that

\[
s'_{s} \approx s'((nK_D^{\pm}) + \nabla_ks'((k))|_{k=nK_D^{\pm}} - (k - nA) + O(k^2).
\] (27)

Thus, the matrix elements of Eq. (25) can be expressed as follows:

\[
s'_0 \approx 3\ell_0 + iv_f a(A \times p)_z, \quad \text{(28a)}
\]

\[
s'_{-1} \approx -v_f[(p_x - hA_x) - i(p_y - hA_y)], \quad \text{(28b)}
\]

\[
s'_{s} \approx v_f[(p_x + hA_x) + i(p_y + hA_y)], \quad \text{(28c)}
\]

where \(\ell_0 = \ell_0[1 - \frac{\alpha}{\beta}(1 - \rho)]\), \(p = (1 + \epsilon - \beta\tau)p\), and we defined the Fermi velocity \(v_f = 3a_0/2\hbar\) as usual. Finally, we can write the Dirac-like equation for electrons in strained graphene with a Kekulé distorsion as,

\[
\mathcal{H} = \begin{pmatrix} \psi^- & \psi^+ \end{pmatrix},
\]

\[
\mathcal{H} = \begin{pmatrix} \psi_{-} & \psi_{+} \end{pmatrix},
\] (29b)

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where $\psi_{s,v}$ is the wavefunction for sublattice $s \in \{A, B\}$ in the valley $v \in \{+, -\}$ and the Pauli matrices $\sigma_i$, $i \in \{0, x, y, z\}$ are acting in the pseudospin degree of freedom.

The energy eigenvalues of the Hamiltonian (29c) can be obtained analytically for both Kekulé textures. For the Kek-O texture ($\nu = 0$), we obtain the following expression,

$$E^2_{O,\pm} = \psi^2((|p|^2 + \hbar^2|A|^2) + \Delta_0^2(|3\hbar|)^2 + [v_f a(A \times p)_z]^2)$$

$$\pm 2v_f \sqrt{\psi^2\hbar^2(\mathbf{A} \cdot \mathbf{p}) + \Delta_0^2(\psi^2 a^2|\mathbf{A}|^2(\mathbf{p} \times \mathbf{p})_z + 2v_f h\tau_0(\mathbf{A} \times \mathbf{p})_z + \hbar^2(|3\hbar|^2|\mathbf{A}|^2)},$$

which recovers the result for the Kek-O unstrained graphene$^{13}$ and may be evaluated at $(k_x, k_y) = (0, 0)$ to find the condition for keeping the gap$^{35}$,

$$\epsilon < \frac{4|\Delta_0|}{\beta[1(1 + \rho) + 2|\Delta_0|(1 - \rho)]}$$

(31)

as well as its magnitude,

$$E_{\text{Gap}} = 6\hbar_0(|\Delta_0| - \frac{\beta\epsilon}{4}(1 + \rho) - \frac{\beta\epsilon}{2}(1 - \rho)|\Delta_0|)$$

(32)

This characterizes the competition between the Kekulé strength $\Delta_0$, and the magnitude of the applied strain $\epsilon$ to open and close the gap, and suggest a way to control this gap by strain. It has been pointed out that this gap becomes topological$^{5}$ for negative values of $\Delta_0$. Notice that both equations are independent from the strain direction $\theta$, this is a consequence of the approximations made for small strain and low-energy. When the magnitude of strain equals the condition given by Eq. (31), the gap closes and the valence and conduction bands touch in just one point. For greater values of strain, the bands touch in two points (valleys) that split as strain increases. This is shown in the series of plots in Fig. 3(a)-3(b), where the dispersion relations around the center of the Brillouin zone for strained Kek-O graphene are presented. Gray lines are the dispersions for unstrained graphene with Kek-O texture. Blue continuous lines present the curves obtained numerically by calculating the eigenvalues of Eq.(19) while dashed lines are the energies in the low energy approximation of Eq.(30). They correspond to the eigenvalues of the effective Hamiltonian for the Kek-O texture given by,

$$\mathcal{H}_O = \nu_f \mathbf{\sigma} \cdot \mathbf{p} \otimes \tau_0 + \nu f \mathbf{\sigma} \cdot \mathbf{A} \otimes \tau_z$$

$$+ 3\Delta_0 t_0 \sigma_+ \otimes \tau_z + v_f a(a(A \times p)_z \sigma_0 \otimes \tau_y, \sigma_0)$$

(33)

where we have taken $\Delta = \Delta_0$, and used a second set of Pauli matrices $\tau_x, \tau_y, \tau_z$, with a unit matrix $\tau_0$ acting on valley space and defined the velocity $v_f = \Delta_0 v_f$. Notice that the pseudomagnetic vector $A$, as usual, appears as a momentum shift, nevertheless since it does not depend on space it can not give rise to a pseudomagnetic field$^{39-41}$. For the Kek-Y texture ($\nu = \pm 1$), a gapless spectrum remains for all values of Kekulé and strain parameters, with energies given by,

$$E^2_{Y,\pm} = v_f^2(1 + \Delta_0^2)(|\mathbf{p}|^2 + \hbar^2|\mathbf{A}|^2)$$

$$\pm v_f^2 \sqrt{2(1 + \Delta_0^2)^2(|\mathbf{p} + h\mathbf{A}|^4 + |\mathbf{p} - h\mathbf{A}|^4) - 2(|\mathbf{p} + h\mathbf{A}|^2)+|\mathbf{p} - h\mathbf{A}|^2(1 - 6\Delta_0^2 + \Delta_0^4)},$$

(34)

In Fig. 3 we present a comparison between Eq. (30) and Eq. (34), with a calculation obtained from a numerical diagonalization of Eq. (19). The good agreement between both calculations validate our expressions for low-energy.

Finally, by taking $\nu = 1$ and $\Delta = \Delta_0$, we obtain the low-energy effective Hamiltonian for the Kek-Y texture,

$$\mathcal{H}_Y = \nu_f \mathbf{\sigma} \cdot \mathbf{p} \otimes \tau_0 + \nu f \mathbf{\sigma} \cdot \mathbf{A} \otimes \tau_z$$

$$+ v_f \sigma_0 \otimes \mathbf{r} \cdot \mathbf{p} + h v_f \sigma_0 \otimes \mathbf{r} \cdot \mathbf{A}.$$ (35)

An equivalent expression is found for $\nu = -1$ and a complex $\Delta$. When compared with the pure Kekulé effective Hamiltonian$^{13}$, we observe two new terms, both containing $A$. These two terms are $k$-independent and have a Zeeman-like structure, one in the pseudospin quantum number as it contains the product $\mathbf{\sigma} \cdot \mathbf{A}$, and the other in the valley quantum number (proportional to $\mathbf{r} \cdot \mathbf{A}$). The former is the leading term, since it depends linearly on $\epsilon$, while the latter depends on the product of $\epsilon \Delta$. Since the first term contains $\tau_z$, it splits the two valleys by moving each cone in opposite directions away from the center $\Gamma$ of the superlattice Brillouin zone, as shown in Fig.3 (d-f). The second term has a similar effect but in
pseudospin space, nevertheless for modest values of strain and Kekulé distortion it can be neglected. Although the first term is proportional to $\tau_2$ and the second is proportional to $\sigma_3$, both preserve the valley and pseudospin energy degeneracy.

IV. CONCLUSIONS

We studied the effects upon the electronic properties of a space-independent strain in different types of Kekulé-patterns in graphene. For the Kek-O type, moderated values of strain preserve the gap although the size is changed. Above a certain strain threshold value, the gaps close leaving a two-Dirac-cones dispersion. For the Kek-Y type, strain splits the valleys along the direction of applied strain. However, as the valleys were folded before by the Kekulé pattern, it turns out that the distance in reciprocal space of the valleys is much closer than in pure graphene. This suggest that strain is useful to control the degree of intervalley scattering in Kekulé patterns. We also provided a low-energy Dirac effective Hamiltonian, which presents a Zeeman-like coupling between pseudospin and valleys to the pseudomagnetic vectorial potential.

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