

Electronic structure of multilayer graphene with arbitrary stackings

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Stacking geometry in multilayer graphene (MLG) provides an interesting degree of freedom to engineer its electronic structure near the Fermi level, wherein the linear bands in single layer graphene could retain or evolve into parabolic or flat bands. Using a tight-binding model, we carried out a detailed analytical analysis of the electronic band structures for arbitrarily stacked MLGs. We show that their low-energy band dispersions near the Fermi level may be deduced from its substacks in isolation. The analytical solutions of the momenta with zero eigenvalue for an AA stacking allow us to generalize the results of the zero-energy momenta for arbitrarily stacked MLGs. Moreover, we find that an interplay of parallel and rhombohedral stacking allows for flat band engineering and enhancement in arbitrarily stacked MLG. The existence of enhanced flat bands in our discussed arbitrarily stacked MLGs might offer another interesting platform for exploring the flat band physics and possible flat band properties, like superconductivity, in graphene systems beyond the twisted bilayer graphene and simpler stacking orders.

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I. INTRODUCTION

The electronic properties of multilayer graphene are fundamentally determined by its stacking geometry, which controls the band structure near the Fermi level. While single-layer graphene features massless Dirac fermions with a linear dispersion [1], multilayer graphene systems exhibit dramatically different behaviors depending on their stacking order and layer number. Early theoretical and experimental studies established that Bernal (AB), rhombohedral (ABC), and parallel (AA) stackings each produce distinct electronic structures [2–5]. Moreover, the nature of charge carriers in few-layer graphene is highly sensitive to both the number of layers and the stacking geometry, making the possibility of analyzing a general arbitrary multilayer stack challenging. Rhombohedral stacking is particularly notable for generating flat bands at low energies, characterized by vanishing Fermi velocity and enhanced density of states. These flat bands play a central role in promoting strong electron-electron correlations and have become a key ingredient for realizing exotic quantum phases including superconductivity [6].

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The discovery of superconductivity in magic-angle twisted bilayer graphene has generated intense interest in flat band engineering as a route to unconventional superconductivity [7,8]. When graphene layers are twisted at specific magic angles (the first being $\theta \approx 1.1^\circ$), moiré superlattices form with isolated flat bands that support Mott insulating states and superconducting domes reminiscent of high- T_c cuprates. This paradigm has been extended to multilayer systems; for example, magic-angle twisted multilayer graphene ($N = 3, 4$, and 5 layers) forms a robust family of moiré superconductors, revealing that flat bands are a common feature but with important variations between even and odd layer numbers [9]. Moreover, gate-tunable superconductivity in ABC-trilayer graphene/hexagonal boron nitride systems have been observed, showing Mott insulating states and superconducting domes that can be continuously tuned via displacement fields [10]. More remarkably, superconductivity has been observed in rhombohedral trilayer graphene without moiré effects, demonstrating that crystalline stacking order alone can generate the necessary conditions for superconductivity [11]. Most recently, signatures of chiral superconductivity in rhombohedral tetra- and pentalayer graphene with transition temperatures up to 300 mK, featuring time-reversal symmetry breaking and magnetic hysteresis hallmarks of unconventional pairing, have been observed [12]. Hence, multilayer graphene has emerged as a versatile platform for exploring correlated electron physics and unconventional superconductivity. To access the full spectrum of electronic properties multilayer graphene offers, however, requires an analysis of completely arbitrary stacking. In doing so, one could predict and engineer a generalized stack to fit their electronic purposes. Understanding how different stacking configurations produce flat bands and influence the electronic properties at the Fermi level is therefore crucial for identifying and designing new foundations for correlated phenomena and superconductivity in graphene systems.

In this work, we carry out an analytical and computational study of the electronic band structures of arbitrarily stacked multilayer graphene (MLG) using a tight-binding model. Stacking sequence in MLG offers a degree of freedom to tune its electronic band dispersions. Within nearest-neighbor interactions (hopping), our Hamiltonian takes on a relatively simple form and the low-energy band dispersions near the K and K' points are calculated. The solutions to pure parallel (AA) and Bernal (AB) stackings, along with the system of (transcendental) equations for ABC stacking, will be derived first. We will then investigate MLG with stacking fault by embedding a certain type of pure stack (e.g., AA) into another type of pure stack (e.g., AB). For MLGs with pure AA substacks, the linear bands persist with the crossing points shifted to other k points other than K and K' . We find an analytical solution to predict the locations of these k points. Furthermore, we will show the robustness of the flat bands in arbitrarily stacked MLGs, which are related to the embedded ABC substacks. The obtained electronic band dispersions are further confirmed by first-principles calculations. Our study shows that the electronic properties of MLGs with an arbitrary stacking sequence may be deduced from its substacks considered in isolation, enabling an interesting design of the desired electronic structures in MLGs.

The paper is organized as follows: In Sec. II, we briefly introduce the tight-binding model used in this work. In Sec. III, we present detailed results for single-layer graphene and multilayer graphene. A conclusion is given in Sec. IV.

II. METHOD

We use a tight-binding method with nearest-neighbor hopping, treating each atomic site as a basis state and constructing our Hamiltonian so that if i and j are neighboring sites, then $\langle i|H|j \rangle = t$ and all non-neighboring hopping integrals are zero [13]. This method has been well received for producing accurate results for many physical systems [14, 15]. For graphene, we only consider the interactions between the $2p_z$ orbitals, since they give rise to the strongest hopping. Our parameters normalize $\hbar = 1$ and $a \approx 1.42 \text{ \AA}$ is the intralayer nearest-neighbor distance, with $t = 3 \text{ eV}$. For MLGs, we only consider the interlayer hopping when two carbon atoms are on top of each other. We set this interlayer hopping term $t_\perp = \frac{t}{10} = 0.3 \text{ eV}$. Our energy units will be in eV (based on the hopping parameters) and momentum units in $\frac{1}{a}$, which are included in the figures. First-principles

calculations based on density functional theory (DFT) are also performed using QUANTUM ESPRESSO code [16] with local density approximation. Norm conserving pseudopotentials for carbon have been adopted. A $36 \times 36 \times 1$ Monkhorst-Pack uniform k -grid and cutoff energy of 90 Ry have been employed.

III. RESULTS AND DISCUSSION

We will first review the basic properties of single-layer graphene and certain types of graphene stacking. We then investigate the MLGs with an arbitrary stacking sequence.

A. Single-layer graphene

As a hexagonal lattice, monolayer graphene has a primitive unit cell of two carbon atoms denoted by a and b . Each carbon atom has three nearest-neighbor interactions; we label nearest-neighboring atoms to have electron annihilation operators $a_{\vec{R}}$ and $b_{\vec{R}+\vec{r}_i}$, where $\vec{r}_i$ denotes translation vectors to the nearest neighbors, so that the Hamiltonian may be constructed as [17]

$$H = -t \sum_{\vec{R}, i} a_{\vec{R}}^\dagger b_{\vec{R}+\vec{r}_i} + \text{H.c.} \quad (1)$$

Converting to the Bloch bases with annihilation operators for a given momentum $a_{\vec{k}}$ and $b_{\vec{k}}$ defined by

$$a_{\vec{R}} = \frac{1}{\sqrt{N}} \sum_{\vec{k}} a_{\vec{k}} e^{i\vec{k} \cdot \vec{R}}, \quad b_{\vec{R}} = \frac{1}{\sqrt{N}} \sum_{\vec{k}} b_{\vec{k}} e^{i\vec{k} \cdot \vec{R}} \quad (2)$$

gives us [18]

$$H = -t \sum_i \sum_{\vec{k}} a_{\vec{k}}^\dagger b_{\vec{k}} e^{i\vec{k} \cdot \vec{r}_i} + \text{H.c.}, \quad (3)$$

which in matrix form gives

$$H(\vec{k}) = \begin{pmatrix} 0 & -t \sum_i e^{i\vec{k} \cdot \vec{r}_i} \\ -t \sum_i e^{-i\vec{k} \cdot \vec{r}_i} & 0 \end{pmatrix}. \quad (4)$$

Since we are working for a given $\vec{k}$, we will omit explicitly giving the $\vec{k}$ dependence in our bases (there is, of course, $\vec{k}$ dependence on our Hamiltonian components, however) and refer to the Bloch bases as simply a and b . The dispersion relation for $\vec{k} = \begin{pmatrix} k_x \\ k_y \end{pmatrix}$ can be shown to be [19,20]

$$\epsilon_{\pm, \vec{k}} = \pm t \sqrt{3 + 2 \cos(\sqrt{3} k_y a) + 4 \cos\left(\frac{\sqrt{3} k_y a}{2}\right) \cos\left(\frac{3 k_x a}{2}\right)}, \quad (5)$$

which is plotted in Fig. 1(a). Note how the low-energy regions (purple) form a hexagon. We have sketched the points of zero energy, which are also the corners of the first Brillouin zone. We may choose K and K' as shown in the figure so that all the other zero-energy points are connected to these two points by reciprocal lattice vectors.

For monolayer graphene, the two bands cross at the Fermi level, suggesting that low-energy analysis should be done near the K or K' points. We will choose K . Specifically, we shift the origin to be at $\vec{K}$ and measure the momentum relative to $\vec{K}$, which we will call $\vec{p} = \vec{k} - \vec{K}$. Performing a linear expansion $h(\vec{K} + \vec{p})$ we will, defining $\vec{p} = \begin{pmatrix} p_x \\ p_y \end{pmatrix}$, the Fermi velocity $v = \frac{3ta}{2}$, and $\pi = p_x + ip_y$,

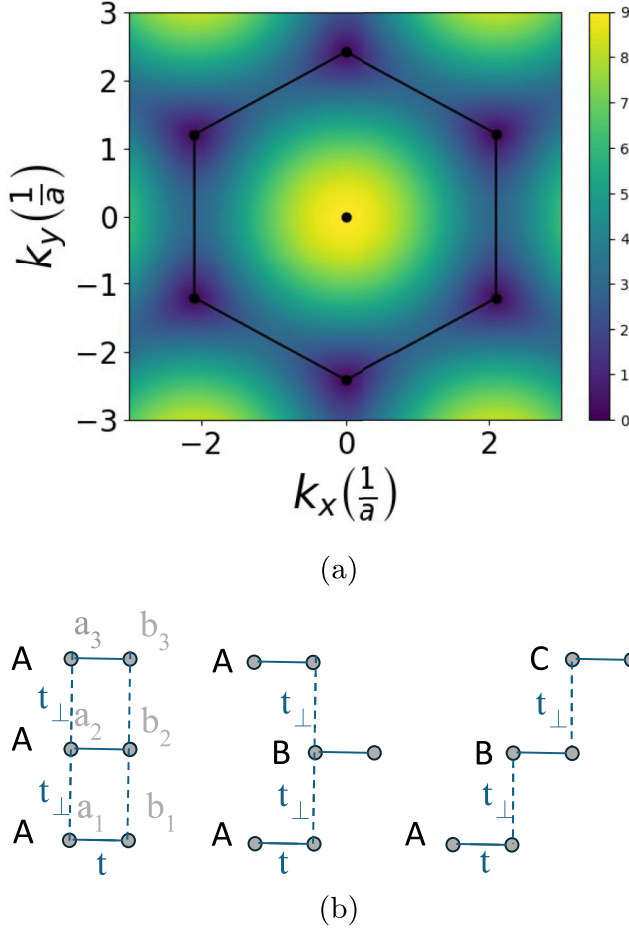


FIG. 1. (a) Contour map of the positive branch of the band dispersion for monolayer graphene in the whole hexagonal Brillouin zone. The corners of the hexagon are the points of zero energy. Examples of the K and K' points have been shown. (b) Schematic of AAA, ABA, and ABC graphene stacking geometry in the Bloch basis. The a and b bases (gray), hopping integrals (cyan), and stacking letters (black) have been shown, which naturally construct the Hamiltonian.

arrive at, upon performing a global gauge transformation [18],

$$H(\vec{p}) = \begin{pmatrix} 0 & v\pi^\dagger \\ v\pi & 0 \end{pmatrix}, \quad (6)$$

where we recognize the two-dimensional massless Dirac Hamiltonian [3]:

$$H = v\sigma \cdot \vec{p}. \quad (7)$$

The dispersion relation, which is

$$\epsilon_{\pm, \vec{p}} = \pm v|\vec{p}|, \quad (8)$$

is notably linear. This is consistent with the band structure of the exact dispersion relation near the K and K' points.

B. Multilayer graphene

Graphene stacking is characterized by how we orient each sheet relative to the one below it, which working with a and b is understood as where we stack each successive a_{i+1} and b_{i+1} sites onto the a_i and b_i sites. We have three options. We may orient the a_{i+1} site onto the b_i site, or orient each a_{i+1} and b_{i+1} onto a_i and b_i , respectively, or orient b_{i+1} onto a_i . These three choices give rise to three stacking orientations A, B, and C, as shown in Fig. 1(b). In general, we can choose the first stack in our sequence to be of type A, which is done without loss of generality. Then, among the above stacking options, AB, BC, and CA all refer to the first stacking option; AA, BB, and CC all refer to the second stacking option; and AC, CB, and BA all refer to the third stacking option. Three different stackings for trilayer graphene have been sketched in Fig. 1(b). We will first consider a general, arbitrary stack and then apply it to the well-known cases. For a given momentum, we omit the $\vec{k}$ subscripts in our creation and annihilation operators (like we did for the Bloch bases), assuming it to be implied. We thus have

$$H = \left(v\pi^\dagger \sum_{i=1}^N b_i^\dagger a_i + t_\perp \sum_{j=1}^{N-1} (\alpha_j a_{j+1}^\dagger b_j + \beta_j (a_{j+1}^\dagger a_j + b_{j+1}^\dagger b_j) + \gamma_j b_{j+1}^\dagger a_j) \right) + \text{H.c.} \quad (9)$$

In matrix form, we have

$$H(\vec{p}) = t_\perp \begin{pmatrix} 0 & f\pi^\dagger & \beta_1 & \gamma_1 & 0 & 0 & \cdots & 0 & 0 \\ f\pi & 0 & \alpha_1 & \beta_1 & 0 & 0 & \cdots & 0 & 0 \\ \beta_1 & \alpha_1 & 0 & f\pi^\dagger & \beta_2 & \gamma_2 & \cdots & 0 & 0 \\ \gamma_1 & \beta_1 & f\pi & 0 & \alpha_2 & \beta_2 & \cdots & 0 & 0 \\ 0 & 0 & \beta_2 & \alpha_2 & 0 & f\pi^\dagger & \cdots & 0 & 0 \\ 0 & 0 & \gamma_2 & \beta_2 & f\pi & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & f\pi^\dagger \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & f\pi & 0 \end{pmatrix}, \quad (10)$$

where $f = \frac{v}{t_\perp}$ and we have defined $(\alpha_i, \beta_i, \gamma_i)$ to follow the relations

$$\alpha_j \beta_j = 0, \quad (11)$$

$$\beta_j \gamma_j = 0, \quad (12)$$

$$\gamma_j \alpha_j = 0, \quad (13)$$

$$\alpha_j + \beta_j + \gamma_j = 1. \quad (14)$$

In other words, $(\alpha_j, \beta_j, \gamma_j) \in \{(1, 0, 0), (0, 1, 0), (0, 0, 1)\}$, wherein AB, BC, CA stacking refers to the $(1, 0, 0)$ solution; AA, BB, CC stacking refers to the $(0, 1, 0)$ solution; and BA, CB, AC stacking refers to the $(0, 0, 1)$ solution. There are three well-studied stacking structures. The first we will consider is AA stacking, what we will call parallel stacking, where we have a stacking sequence

AAAA ... given by the Hamiltonian

$$H_{AA} = \begin{pmatrix} 0 & v\pi^\dagger & t_\perp & 0 & 0 & 0 & \cdots & 0 & 0 \\ v\pi & 0 & 0 & t_\perp & 0 & 0 & \cdots & 0 & 0 \\ t_\perp & 0 & 0 & v\pi^\dagger & t_\perp & 0 & \cdots & 0 & 0 \\ 0 & t_\perp & v\pi & 0 & 0 & t_\perp & \cdots & 0 & 0 \\ 0 & 0 & t_\perp & 0 & 0 & v\pi^\dagger & \cdots & 0 & 0 \\ 0 & 0 & 0 & t_\perp & v\pi & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & v\pi^\dagger \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & v\pi & 0 \end{pmatrix}. \quad (15)$$

Upon employing recurrence methods, we reach the dispersion relation [5]

$$\epsilon_{r,\vec{p}}^{\pm,AA} = \pm v|\vec{p}| + 2t_\perp \cos\left(\frac{r\pi}{N+1}\right), \quad (16)$$

where $r \in \{1, 2, 3, \dots, N\}$ and N is the length (number of layers) of our stack. In general, an N -layer stack will have a Hamiltonian with dimensions of $2N \times 2N$. We notice that this is simply a sum of the eigenenergies of the Dirac Hamiltonian and that of the open chain tight-binding model [13]. It is intuitive due to the parallel nature of the stack. Moreover, it will be useful later for comparison to find specifically the momentum values $|\vec{p}|$ for which $\epsilon_{r,\vec{p}}^{\pm,AA} = 0$. They are given by

$$|\vec{p}| = \left| \frac{2t_\perp}{v} \cos\left(\frac{r\pi}{N+1}\right) \right|, \quad (17)$$

where the absolute value on the cosine function is justifiable since our dispersion relation concerns only with $\pm|\vec{p}|$. The dispersion relation for tetralayer (four-layer) AA stacking is plotted in Fig. 2(a). Notice the linear bands that resemble the shifted dispersion relation for monolayer massless Dirac fermions. These shifts generate multiple band crossings at momentum values other than the $\vec{K}$ and $\vec{K}'$ points. These crossings are characteristic of AA stacking, a property that will be insightful in analyzing arbitrary stacking.

For AB stacking, which is referred to as Bernal stacking, we have a stacking sequence ABABAB ..., which is given by the Hamiltonian

$$H_{AB} = \begin{pmatrix} 0 & v\pi^\dagger & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ v\pi & 0 & t_\perp & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & t_\perp & 0 & v\pi^\dagger & 0 & t_\perp & \cdots & 0 & 0 \\ 0 & 0 & v\pi & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & v\pi^\dagger & \cdots & 0 & 0 \\ 0 & 0 & t_\perp & 0 & v\pi & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & v\pi^\dagger \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & v\pi & 0 \end{pmatrix}. \quad (18)$$

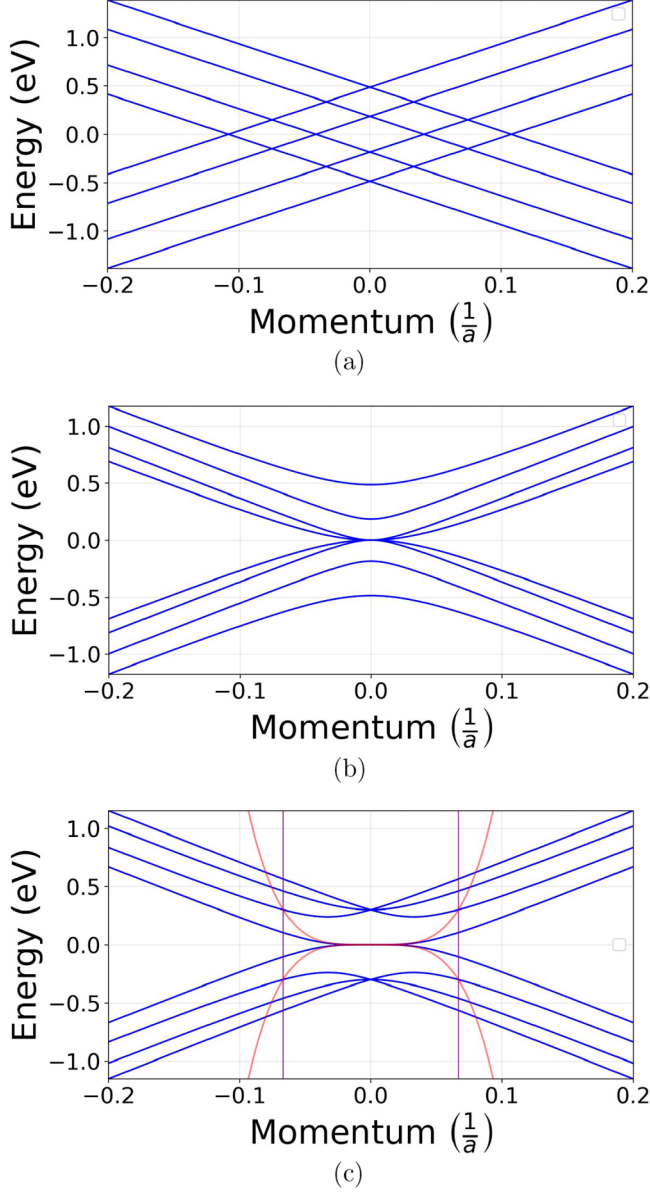


FIG. 2. Calculated electronic band dispersions for (a) tetralayer AA stacked graphene, (b) tetralayer AB stacked graphene, and (c) tetralayer ABC stacked graphene. The approximate low-energy band analytical solution (red) is also shown for comparison in panel (c). Note the accuracy at small momentum. The maximum flat band range, when N is large, is bounded by the momentum values plotted via purple vertical lines.

Upon employing similar recurrence methods for this matrix, we can reach the dispersion relation [5]

$$\epsilon_{r,\vec{p}}^{\pm,AB} = t_{\perp} \cos\left(\frac{r\pi}{N+1}\right) \pm \sqrt{v^2|\vec{p}|^2 + t_{\perp}^2 \cos^2\left(\frac{r\pi}{N+1}\right)}. \quad (19)$$

This equation for tetralayer AB stacking is plotted in Fig. 2(b). The structure of the equation follows the massive Dirac fermion dispersion relation, with parabolic bands at low energies.

Finally, the ABC stacking, denoted by a stacking sequence ABCABCABC ..., is given by the Hamiltonian

$$H_{\text{ABC}} = \begin{pmatrix} 0 & v\pi^\dagger & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ v\pi & 0 & t_\perp & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & t_\perp & 0 & v\pi^\dagger & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & v\pi & 0 & t_\perp & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & t_\perp & 0 & v\pi^\dagger & \cdots & 0 & 0 \\ 0 & 0 & 0 & 0 & v\pi & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & v\pi^\dagger \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & v\pi & 0 \end{pmatrix}. \quad (20)$$

The analytical solution can be represented as a system of two transcendental equations [4]. One of the characteristics of the Hamiltonian, however, is the localized eigenstate that produces a low-energy flat band. We may apply a Schrieffer-Wolf transformation to the Hamiltonian to obtain the low-energy dispersion relation [5,21]

$$\epsilon_{\vec{p}}^{\pm, \text{ABC}} = \pm t_\perp \left(\frac{v|\vec{p}|}{t_\perp} \right)^N. \quad (21)$$

Since the Schrieffer-Wolf transformation is derived from assuming that the energy eigenvalue is much smaller than the elements of the Hamiltonian matrix, define $\Delta|\vec{p}|$ such that

$$t_\perp \left(\frac{v\Delta|\vec{p}|}{t_\perp} \right)^N = t_\perp. \quad (22)$$

The momenta around and greater than $\Delta|\vec{p}|$ are obtained when the Schrieffer-Wolf transformation becomes inaccurate. So, the radius in which this approximation is accurate is given by

$$\Delta|\vec{p}| = \frac{t_\perp}{v}. \quad (23)$$

Moreover, we could also have derived this as $\lim_{N \rightarrow \infty} \left(\frac{v\Delta|\vec{p}|}{t_\perp} \right)^N = 1$, which shows that Eq. (23) also approximates the radius of the flat band in the large layer number N limit. In this limit, at $|\vec{p}| < \Delta|\vec{p}|$, our eigenenergy is almost zero, and at $|\vec{p}| > \Delta|\vec{p}|$, our eigenenergy becomes very large. Note that the localization of this flat band is specifically observed for trilayer ABC graphene and above; we understand that bilayer rhombohedral graphene and bilayer Bernal graphene are the same. Figure 2(c) shows the dispersion relation for tetralayer ABC graphene. Clearly, the flat bands near the Fermi level are present. We have also plotted our approximated flat band dispersion relation in red, which achieves accuracy at low momentum (and therefore low energy) values. As our layer number N becomes large, our approximation also gives a maximum momentum radius of our flat band according to Eq. (23), which we have plotted in purple.

For ABC stacking, the origin of the flat band is due to edge state localization that causes our Hamiltonian to have a particularly low-energy eigenstate solution. For an N -layer ABC stacking specifically, there exists only two sites in the Bloch bases that have no interlayer hopping; all other sites do. These are a_1 and b_N . Occupation of other sites would lead to higher-energy eigenstates due to the energy associated with interlayer hopping, so a_1 and b_N serve as the basis for the low-energy domain for our Schrieffer-Wolf transformation. The low-energy charge density distribution for tetralayer ABC stacking is plotted in Fig. 3. Specifically, the eigenstates of our Hamiltonian give

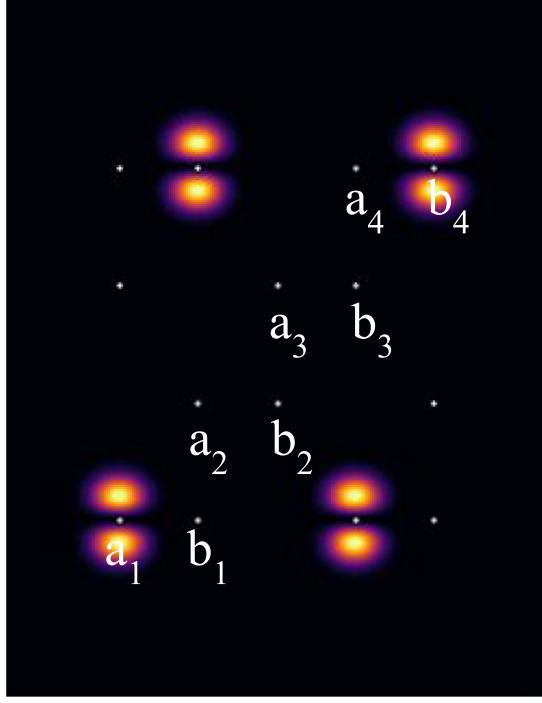


FIG. 3. The low-energy charge density for tetralayer ABC stacked graphene with sufficiently low momentum in the flat band. The stack is copied over horizontally to show the periodic nature of the crystal lattice. Each dot represents a Bloch site (labeled in a picture for a given stack), and the electronic π orbitals are highlighted with a given intensity based on the eigenvectors to our Hamiltonian. Note the edge state localization at sites a_1 and b_4 . These are the low-energy basis states in our Schrieffer-Wolf transform.

the amplitudes for which electrons may be localized at any given site, according to the tight-binding model. There is clear localization on specifically the edge states, where the amount of hopping energy is minimal (there is no interlayer hopping). This minimizes energy, which explains the flat band.

C. Multilayer graphene with arbitrary stackings

We now consider a multilayer graphene with a generalized stacking, which we call arbitrary stacking. Excluding twisting, arbitrary stacking can be represented by a string of the letters A, B, and C that will represent the relative orientation of each graphene layer. The cases of AA, AB, and ABC stacking are special cases of this form of stacking.

Each well-understood stacking has its own properties [5]. We may understand arbitrary stacking as an embedding of the stacking sequences for which we have studied earlier. The most studied cases are those of stacking faults, where we, in a sequence of parallel, Bernal, or rhombohedral stacking, embed a small sequence of another one of the three common structures [22]. For example, the sequence ABABABBABAB is one such fault, where we have embedded a parallel sequence within a Bernal sequence; the sequence ABCABCBCABCABC is another such fault, where we have embedded a Bernal sequence within a rhombohedral sequence. We will investigate the properties of the three stacking sequences and see how they evolve when we employ arbitrary stacking.

First, we observe the emergence of the flat band. Figure 4 shows the dispersion relation for embedding ABC stacking into the parallel and Bernal stacking, respectively, along with the respective flat band for the embedded substacks; we see a striking resemblance between a flat band for our embedded ABC stacking and that of pure ABC stacking. It is thus possible to induce a flat band

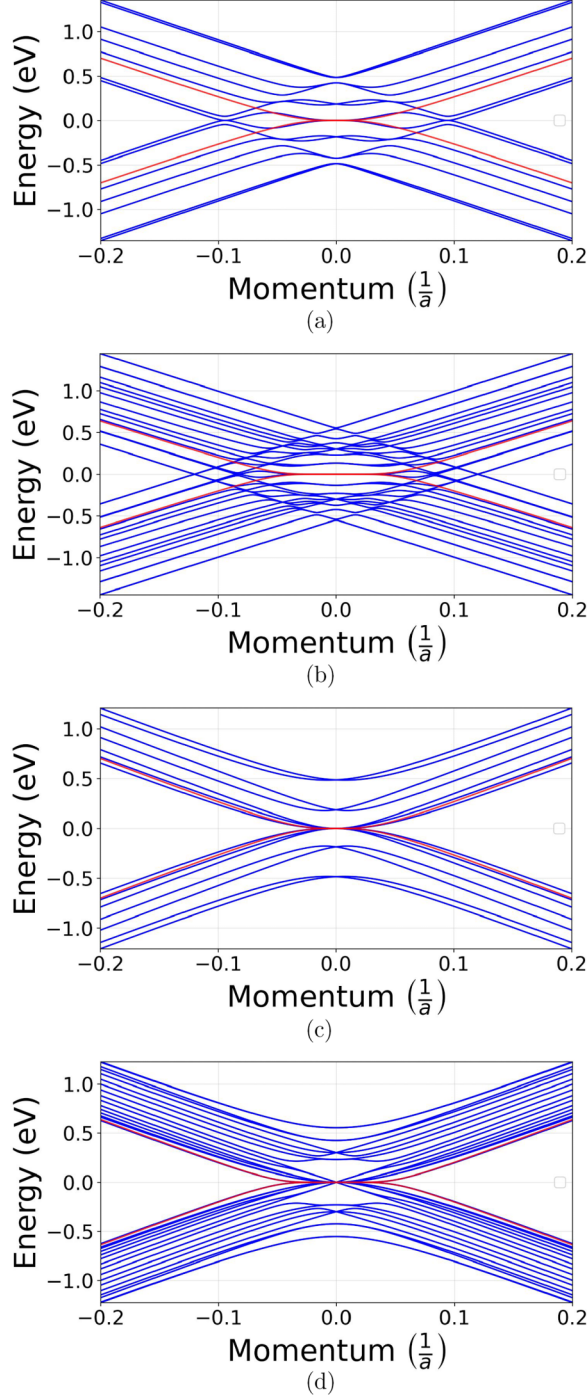


FIG. 4. (a) Band dispersions for AAABCCC (blue). The dispersion for an ABC trilayer graphene is shown in red for comparison. Note how the flat band flattens the points of zero energy. (b) Band dispersions for AAAAAABCABCCCCC (blue). The band dispersions for ABCABCB are shown in red. (c) Band dispersions for ABABCBC (blue). The band dispersions for ABC trilayer graphene are shown in red. (d) Band dispersions for BABABABCBCBCBCB (blue) and for ABCABCB (red).

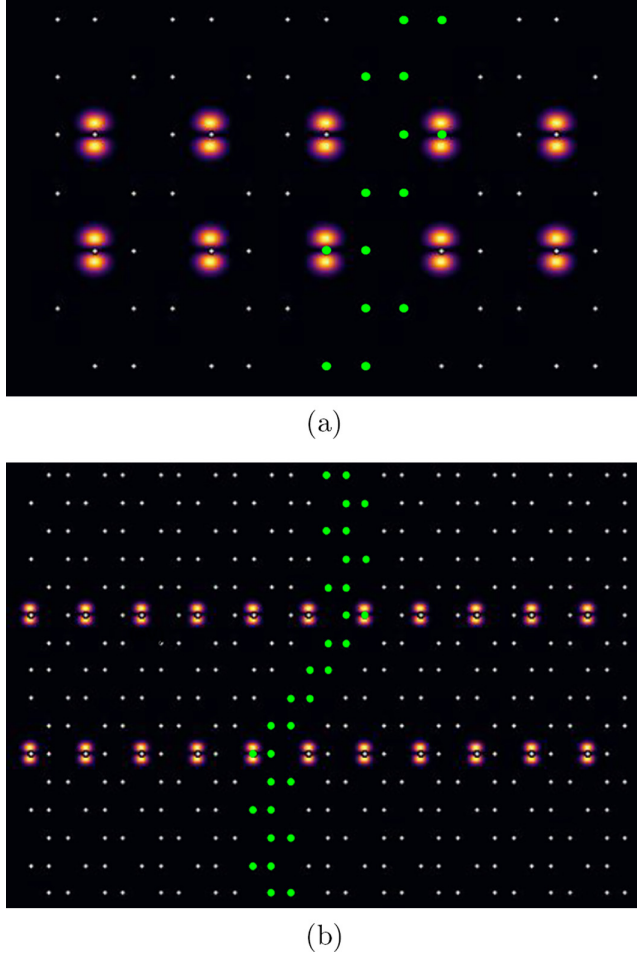


FIG. 5. Sufficiently low-energy flat band eigenstate for (a) ABABCBC and (b) BABABABCABCBCBCB. For clarity, we have highlighted the stacking sequence of the carbon atoms using green dots. Note the localization at the edges of the embedded ABC substack. We do not see this for an ABC substack embedded within a parallel stacking.

within parallel or Bernal stacking by inserting a rhombohedral stacking fault. This suggests the principle of decomposing a stack into components to analyze its properties, since the existence of ABC stacking within an arbitrary stack seems to be directly linked with the existence of a flat band.

Moreover, for embedding a rhombohedral substack into a Bernal stacking, it seems that we maintain the edge state localization within the ABC substack. This behavior is shown in Figs. 5(a) and 5(b), corresponding to the charge densities for the flat band exhibited by the dispersion relations plotted in Figs. 4(c) and 4(d), respectively. For reference, we show in green the pattern followed by the stacking sequence. We have edge state localization, not at the edges of the stack, but instead at the edges of the ABC substack. We do not see the same localization when we embed an ABC substack into a parallel stacking. This is because, for AA stacking embedded with an ABC stack, the edges of the ABC substack no longer preserve the isolated sites with only intralayer coupling. Instead, we are forced to have interlayer coupling for the ABC edge sites, which no longer makes them necessarily low energy. For ABC embedded Bernal stacking, however, the edge states still preserve their low-energy property.

One notable property of the AB stacking with an ABC fault is the presence of both a linear and a flat band. As we have already shown, a flat band can be induced by embedding an ABC stack into any arbitrary graphene stack. Moreover, Eq. (19) can exhibit linear bands when N is odd, allowing $r = \frac{N+1}{2}$ to be an integer so that $t_\perp \cos(\frac{r\pi}{N+1}) = 0$. This creates a linear band $\epsilon_{\frac{N+1}{2}, \vec{p}}^{\pm, AB} = \pm v|\vec{p}|$, which is exactly the same as Eq. (8). It is understood that flat bands, on the scale induced by large ABC stacks, are indicative of strongly correlated electronic systems. Furthermore, the linear band of Eq. (8) represents the existence of massless Dirac fermions. For certain AB stacking embedded with ABC stacking, the possibility to simultaneously maintain a linear band and induce a flat band implies the coexistence of strongly correlated electrons with massless Dirac fermions. Thus, these stacks could be viable in providing insight into the interactions of these particles.

Figures 4(a) and 4(b) show the dispersion relations for AA stacking with an ABC fault. In AA stacking, we have multiple zero-energy points that are understood as rings about the Dirac point. Electrons will fill these regions first before moving upward in energy [23]. Figures 4(c) and 4(d) show the dispersion relations for AB stacking with an ABC fault. In AB stacking, the zero-energy locations occur only at the Dirac point. We may induce this property of AA stacking into nonparallel stacking by means of stacking faults. Notice that the stacks that include some parallel stacking are exclusively the ones that have band crossings at nonzero $|\vec{p}|$ values from the $\vec{K}$, namely, Figs. 4(a) and 4(b). In fact, we can make an analytical statement about the direct linkage between AA stacking and these nontrivial band crossings, moreover finding the exact $\vec{p}$ for which these occur. Zero eigenvalues correspond to our stacking matrix

$$H(\vec{p}) = t_\perp \begin{pmatrix} 0 & f\pi^\dagger & \beta_1 & \gamma_1 & 0 & 0 & \cdots & 0 & 0 \\ f\pi & 0 & \alpha_1 & \beta_1 & 0 & 0 & \cdots & 0 & 0 \\ \beta_1 & \alpha_1 & 0 & f\pi^\dagger & \beta_2 & \gamma_2 & \cdots & 0 & 0 \\ \gamma_1 & \beta_1 & f\pi & 0 & \alpha_2 & \beta_2 & \cdots & 0 & 0 \\ 0 & 0 & \beta_2 & \alpha_2 & 0 & f\pi^\dagger & \cdots & 0 & 0 \\ 0 & 0 & \gamma_2 & \beta_2 & f\pi & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & f\pi^\dagger \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & f\pi & 0 \end{pmatrix} \quad (24)$$

having zero determinant. Then, define χ_i for $i \in \{1, 2, 3, \dots, 2N\}$ to be the determinant from rows and columns i to $2N$, or in other words, the determinant of the bottom right submatrix of dimensions $(2N - i + 1) \times (2N - i + 1)$ (working from left to right and top to bottom, this submatrix would be constructed by taking the i th row and column and everything onward). We hence establish by definition

$$\chi_{2N-1} = -v^2|\vec{p}|^2. \quad (25)$$

Let us work for $k \in \{1, 2, 3, \dots, N-1\}$. Then, χ_{2k-1} may be interpreted as the determinant of a substack of $N - k + 1$ layers, starting from the bottom of our original stack of N layers. If $\alpha_k = 1$, we have

$$\chi_{2k-1} = -v^2|\vec{p}|^2 \chi_{2(k+1)-1}, \quad (26)$$

where we use the fact that if a matrix has an entire column of zeros, its determinant is zero. If $\gamma_k = 1$, we similarly have

$$\chi_{2k-1} = -v^2|\vec{p}|^2 \chi_{2(k+1)-1}. \quad (27)$$

We see that, for a stack whose top two sheets are connected by an AC or AB connection (so that there is a shift between them), the determinant of the original substack, denoted by χ_{2k-1} , is 0 for

$|\vec{p}| \neq 0$ if and only if its determinant taking the topmost sheet off, denoted by $\chi_{2(k+1)-1}$, is also 0. Then, having the determinant be 0 is impossible if we only have Bernal and rhombohedral stacking as the recurrence relation has shown (the base case, for monolayer graphene, is always nonzero for $|\vec{p}| \neq 0$). Essentially, we have shown that the determinant of a stack of size N represented by a string where adjacent characters are different (ABABABC is one such string, ABBAB is not) is equal to

$$\det(H) = (-1)^N v^{2N} |\vec{p}|^{2N}, \quad (28)$$

which is 0 if and only if $|\vec{p}| = 0$. AA stacking does not follow such a simple recurrence relation. Hence, it is possible for it to induce multiple Dirac points. For a substack that is on top an AA pattern, which would be the $\beta_k = 1$ case, we can write in block matrix form

$$H = \begin{pmatrix} \mathbf{M} & t_{\perp} \mathbf{J} \\ t_{\perp} \mathbf{J}^T & \mathbf{S} \end{pmatrix}, \quad (29)$$

where $\mathbf{M}$ is the Hamiltonian for monolayer graphene and $\mathbf{S}$ is the Hamiltonian for the substack if we take the top layer (connected by an AA stacking connection) off. $\mathbf{J}$ is defined as

$$\mathbf{J} = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \end{pmatrix} \quad (30)$$

to keep the matrix square. For such a block matrix, we may use the determinant formula [24]

$$\det(H) = \det(\mathbf{M}) \det(\mathbf{S} - t_{\perp}^2 \mathbf{J}^T \mathbf{M}^{-1} \mathbf{J}), \quad (31)$$

which implies that $\det(H) = 0$ if and only if $\det(\mathbf{S} - t_{\perp}^2 \mathbf{J}^T \mathbf{M}^{-1} \mathbf{J}) = 0$.

Of course,

$$\mathbf{M}^{-1} = \frac{1}{v^2 |\vec{p}|^2} \begin{pmatrix} 0 & v\pi^{\dagger} \\ v\pi & 0 \end{pmatrix}, \quad (32)$$

meaning that

$$t_{\perp}^2 \mathbf{J}^T \mathbf{M}^{-1} \mathbf{J} = \frac{t_{\perp}^2}{v^2 |\vec{p}|^2} \begin{pmatrix} 0 & v\pi^{\dagger} & 0 & 0 & \cdots & 0 \\ v\pi & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 0 \end{pmatrix}. \quad (33)$$

If we now assume the next sequence has $\beta_{k-1} = 0$, then $t_{\perp}^2 \mathbf{J}^T \mathbf{M}^{-1} \mathbf{J}$ can be written in the matrix form:

$$\mathbf{S} - t_{\perp}^2 \mathbf{J}^T \mathbf{M}^{-1} \mathbf{J} = \begin{pmatrix} 0 & \left(1 - \frac{t_{\perp}^2}{v^2 |\vec{p}|^2}\right) v\pi^{\dagger} & 0 & \gamma_{k+1} t_{\perp} & \cdots & 0 \\ \left(1 - \frac{t_{\perp}^2}{v^2 |\vec{p}|^2}\right) v\pi & 0 & \alpha_{k+1} t_{\perp} & 0 & \cdots & 0 \\ 0 & \alpha_{k+1} t_{\perp} & 0 & v\pi^{\dagger} & \cdots & 0 \\ \gamma_{k+1} t_{\perp} & 0 & v\pi & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 0 \end{pmatrix}, \quad (34)$$

whose determinant we gather from the same method we used to derive Eqs. (26) and (27) to be

$$\det(\mathbf{S} - t_{\perp}^2 \mathbf{J}^T \mathbf{M}^{-1} \mathbf{J}) = - \left(1 - \frac{t_{\perp}^2}{v^2 |\vec{p}|^2} \right)^2 v^2 |\vec{p}|^2 \chi_{2(k+2)-1}. \quad (35)$$

This generates a zero determinant at $|\vec{p}| \neq 0$, namely, $|\vec{p}| = \frac{t_{\perp}}{v}$. We may also generalize this to L parallel connections (which is to say, we embed a length $L + 1 = N$ parallel stacks). In general, this determinant is 0 if we have a 2×2 block of zeros in the top left. Define

$$Q_0(\vec{p}) = 0, \quad (36)$$

$$Q_{n+1}(\vec{p}) = \frac{t_{\perp}^2}{(1 - Q_n(\vec{p}))v^2 |\vec{p}|^2}. \quad (37)$$

We would like to show inductively that we can solve for $|\vec{p}| \neq 0$ that gives zero determinant by setting

$$Q_L(\vec{p}) = 1. \quad (38)$$

As we discussed earlier, this only happens if in the place of top left monolayer of the resultant difference is a matrix of zeros. In general, we would have our matrix whose determinant we set to 0 to be

$$\begin{pmatrix} \mathbf{M} & t_{\perp} \mathbf{J} \\ t_{\perp} \mathbf{J}^T & \mathbf{S} \end{pmatrix} = \begin{pmatrix} 0 & (1 - Q_n(\vec{p}))v\pi^{\dagger} & \beta t_{\perp} & \gamma t_{\perp} & \cdots & 0 \\ (1 - Q_n(\vec{p}))v\pi & 0 & \alpha t_{\perp} & \beta t_{\perp} & \cdots & 0 \\ \beta t_{\perp} & \alpha t_{\perp} & 0 & v\pi^{\dagger} & \cdots & 0 \\ \gamma t_{\perp} & \beta t_{\perp} & v\pi & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 0 \end{pmatrix}, \quad (39)$$

since our inductive step requires us to assume this is true. More concretely, we are requiring that the above matrix has zero determinant for the $\beta = 0$ case, at the end of the N -layer stack where $L = N - 1$, which implies Eq. (38). Essentially, our mathematical formula that creates a subproblem to zero the determinant of $\mathbf{S} - t_{\perp}^2 \mathbf{J}^T \mathbf{M}^{-1} \mathbf{J}$ essentially induces an effective momentum element $v\pi \mapsto (1 - Q_n(\vec{p}))v\pi$, which we need to zero at $\alpha = 1$ or $\gamma = 1$ connections. To proceed with induction, note we have already solved a base case for for we have only one parallel connection. We take the $\beta = 1$ case and we solve with the formula given in Eq. (31), noting that

$$\mathbf{M}^{-1} = \frac{1}{((1 - Q_n(\vec{p}))v)^2 |\vec{p}|^2} \begin{pmatrix} 0 & (1 - Q_n(\vec{p}))v\pi^{\dagger} \\ (1 - Q_n(\vec{p}))v\pi & 0 \end{pmatrix}. \quad (40)$$

Calculating $\mathbf{S} - t_{\perp}^2 \mathbf{J}^T \mathbf{M}^{-1} \mathbf{J}$, we therefore need to zero the determinant of

$$\begin{pmatrix} 0 & \left(1 - \frac{t_{\perp}^2}{(1 - Q_n(\vec{p}))v^2 |\vec{p}|^2}\right)v\pi^{\dagger} & \beta_{-} t_{\perp} & \gamma_{-} t_{\perp} & \cdots & 0 \\ \left(1 - \frac{t_{\perp}^2}{(1 - Q_n(\vec{p}))v^2 |\vec{p}|^2}\right)v\pi & 0 & \alpha_{-} t_{\perp} & \beta_{-} t_{\perp} & \cdots & 0 \\ \beta_{-} t_{\perp} & \alpha_{-} t_{\perp} & 0 & v\pi^{\dagger} & \cdots & 0 \\ \gamma_{-} t_{\perp} & \beta_{-} t_{\perp} & v\pi & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 0 \end{pmatrix}, \quad (41)$$

where $(\alpha_-, \beta_-, \gamma_-)$ precedes (α, β, γ) . This is equal to by definition

$$\begin{pmatrix} 0 & (1 - Q_{n+1}(\vec{p}))v\pi^\dagger & \beta_-t_\perp & \gamma_-t_\perp & \cdots & 0 \\ (1 - Q_{n+1}(\vec{p}))v\pi & 0 & \alpha_-t_\perp & \beta_-t_\perp & \cdots & 0 \\ \beta_-t_\perp & \alpha_-t_\perp & 0 & v\pi^\dagger & \cdots & 0 \\ \gamma_-t_\perp & \beta_-t_\perp & v\pi & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 0 \end{pmatrix}, \quad (42)$$

which thus completes the inductive step. To solve this recurrence, we define $x = \frac{v|\vec{p}|}{t_\perp}$, and $f_n(x) = 1 - Q_n(\vec{p})$, which gives us

$$f_{n+1}(x) = 1 - \frac{1}{f_n(x)x^2}. \quad (43)$$

Our goal now is to find the roots of $f_L(x)$. We note our recurrence can be written as

$$xf_{n+1}(x) = x - \frac{1}{f_n(x)x}. \quad (44)$$

We then consider Chebyshev polynomials of the second kind [25]:

$$U_{n+1}(y) = 2yU_n(y) - U_{n-1}(y), \quad (45)$$

and note that this can be written for $y = \frac{x}{2}$ as

$$\frac{U_{n+1}(\frac{x}{2})}{U_n(\frac{x}{2})} = x - \frac{U_{n-1}(\frac{x}{2})}{U_n(\frac{x}{2})}. \quad (46)$$

We would like to show $xf_n(x) = \frac{U_{n+1}(\frac{x}{2})}{U_n(\frac{x}{2})}$. Notice that the recurrence relations are automatically identical. We know $f_0(x) = 1$ from Eq. (36). Since $U_1(x) = 2x$ and $U_0(x) = 1$, we have $\frac{U_1(\frac{x}{2})}{U_0(\frac{x}{2})} = x = xf_0(x)$, so we have verified both the base case and the recurrence relation, which completes the proof. The roots x_r that satisfy $U_D(x_r) = 0$ are given by

$$x_r = \cos\left(\frac{r\pi}{D+1}\right) \quad (47)$$

for $r \in \{1, 2, 3, \dots, D\}$. Then, we may substitute $x = \frac{x_r}{2}$ and $|\vec{p}| = \frac{t_\perp x}{v}$ with $D = L + 1$ so that for $\vec{p}$ to satisfy Eq. (38), it is necessary that

$$|\vec{p}| = 2\frac{t_\perp}{v} \cos\left(\frac{r\pi}{L+2}\right). \quad (48)$$

Since L is the number of connections, it may be more useful to consider the number of layers $N = L + 1$. We have

$$|\vec{p}| = 2\frac{t_\perp}{v} \cos\left(\frac{r\pi}{N+1}\right). \quad (49)$$

Technically, we would also have to exclude the roots of U_L , but they will in fact never show up in our expression, because $\gcd(n, n+1) = 1$ for $n \in \mathbb{Z}^+$. More importantly, we must carefully consider $|\vec{p}| = 0$. We have implicitly assumed this not to be true when we inverted our monolayer graphene block matrix; if $|\vec{p}| = 0$, then our monolayer graphene matrix becomes singular. Moreover, since $xf_n(x) = \frac{U_{n+1}(\frac{x}{2})}{U_n(\frac{x}{2})}$, we would have to exclude $x = 0 \Rightarrow |\vec{p}| = 0$ as a necessary root of $f_N(x)$ anyway. However, Eq. (49) gives $|\vec{p}| = 0$ for odd N . We can do an inductive proof to show that

indeed zero momentum gives zero energy for odd N only. Our strategy for proof will be to try to find nonzero determinant with matrix minors, and then show that we can do so for odd N but not even N . Define the substack, taking off all the layers until we leave the complete AA embed on top to be $\mathbf{S}$. We will now stack an AA bilayer on top:

$$H = \begin{pmatrix} \mathbf{M}_2 & \mathbf{t} \\ \mathbf{t}^T & \mathbf{S}_2 \end{pmatrix}, \quad (50)$$

where

$$\mathbf{M}_2 = \begin{pmatrix} 0 & 0 & t_{\perp} & 0 \\ 0 & 0 & 0 & t_{\perp} \\ t_{\perp} & 0 & 0 & 0 \\ 0 & t_{\perp} & 0 & 0 \end{pmatrix} \quad (51)$$

and

$$\mathbf{t} = \begin{pmatrix} 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 \\ t_{\perp} & 0 & 0 & \cdots & 0 \\ 0 & t_{\perp} & 0 & \cdots & 0 \end{pmatrix}, \quad (52)$$

again, to keep the matrix square. We realize

$$\det(H) = t_{\perp}^4 \det(\mathbf{S}_2), \quad (53)$$

by using the cofactor expansion to calculate the determinant of our Hamiltonian. Essentially, the only possibly nonzero matrix minor is the one that comes from the $t_{\perp}$ elements in $\mathbf{M}_2$. If we took a $t_{\perp}$ element from $\mathbf{t}_2$ instead of $\mathbf{M}_2$, the resultant submatrix would have a column of zeros, which would mean a matrix minor of zero. In doing this, the only nonzero matrix minor would be the determinant of $\mathbf{S}_2$. It would then be trivial to consider $N = 0$ and $N = 1$. Furthermore, if at any point in our recurrence relation $f_n(x) = 0$ for $n < N$, we would have $\mathbf{M}$ become singular (specifically, a 2×2 matrix of zeros), making Eq. (31) invalid. To resolve this, consider that

$$\mathbf{M}_2 = \begin{pmatrix} 0 & 0 & t_{\perp} & 0 \\ 0 & 0 & 0 & t_{\perp} \\ t_{\perp} & 0 & 0 & v\pi^{\dagger} \\ 0 & t_{\perp} & v\pi & 0 \end{pmatrix}. \quad (54)$$

By similar arguments, Eq. (53) holds. This means that the effect in general of having a singular $\mathbf{M}$ at any step will be that the determinant of our Hamiltonian is zero if the determinant $\mathbf{S}_2$ is zero. Notice that if $f_n(x) = 0$, then $f_{n+2}(x) = 1$, which means that our recurrence relation is consistent with this idea and therefore is valid in both sufficiency and completeness. Hence, it is in fact true that every single solution of Eq. (49) conveniently gives zero energy, including the $|\vec{p}| = 0$ solutions. What we have shown is that the zero-energy momenta due to an embedded N -layer AA stack are the exact same momentum for zero energy for the N -layer AA stack itself; Eqs. (49) and (17) are identical for zero-energy eigenvalues [one could, if preferred, also include absolute value signs in Eq. (49) since there is positive and negative symmetry of cosine around $\frac{\pi}{2}$]. Moreover, due to the recurrence relations in Eqs. (26) and (27), Eq. (49) in fact gives every single zero-energy momentum.

Our analysis of completely arbitrary stacking is simply a generalization of stacking faults. It is understood by its derivation that Eq. (49) is true for all arbitrary stacks. In general, our graphene stack is represented by a string of A, B, and C. And every stack can be represented by the stacking of parallel substacks. If we denote some stack to be S , then there exists a sequence S_i

for $i \in \{1, 2, 3, \dots, K\}$ such that

$$S = \bigoplus_{i=1}^P S_i \quad (55)$$

and we guarantee that each S_i is a string of the same letter. Our notation is simply for string concatenation. For example, if S_1 is an AA stack and S_2 is a BB stack, then $S = \bigoplus_{i=1}^2 S_i$ is an AABB stack. Moreover, we establish by necessity that for $j \in \{1, 2, 3, \dots, K-1\}$, S_j and S_{j+1} are of different letters. Then, denote N_i to be the lengths of each parallel stack. For example, BABBBCCCC is composed of B, A, BBB, and CCCC, so in this case $N_i \in \{1, 3, 4\}$. Note how N_i for the stack BABBBCCCC does not contain the element 2. Now, denote $P_i = \{p_{1i}, p_{2i}, p_{3i}, \dots, p_{N_i}\}$ so that

$$p_{ri} = 2 \frac{t_{\perp}}{v} \cos \left(\frac{r_i \pi}{N_i + 1} \right) \quad (56)$$

for $r_i \in \{1, 2, 3, \dots, N_i\}$. Finally, define

$$P_0 = \bigcup_{i=1}^K P_i. \quad (57)$$

Then, $\vec{p}$ gives a zero-energy eigenvalue for our Hamiltonian $H_S(\vec{p})$ if and only if $|\vec{p}| \in P_0$. In other words, if such a $\vec{p}$ gives zero energy for any one of the parallel stacked components S_i of S , then it gives zero energy for S . Equation (56) therefore suggests that the properties of arbitrarily stacked multilayer graphene are determined by considering its substacks in isolation. We have done so by analyzing the role of parallel stacking in an isolated stack. Without parallel stacking, such a phenomenon may also occur in an arbitrary stack consisting of only Bernal and rhombohedral stacking [26]. It has been shown that band structure analysis for low momentum in this case may be done by focusing on the Bernal components in isolation. Hence, the behavior follows our idea above. The electronic properties of arbitrarily stacked multilayer graphene therefore in general appear to be adopted from specific subsequences of its stacking order.

We see also in Fig. 4(a) that embedded ABC substack can induce flatness into these points. We thus have the viability to greatly increase the density of states at the Fermi energy by combining both parallel and rhombohedral stackings. Notably, we will at least be able to double the radius of the region in which our dispersion relation is flat, since the maximum of Eq. (56) as our lower bound implies that in the large N limit

$$\Delta|\vec{p}| \geq \frac{2t_{\perp}}{v}, \quad (58)$$

which is two times that of Eq. (23) pertaining to pure ABC stacking. To concretely show extended flatness, we plot the density of states (DOS) and integrated density of states (IDOS), which quantifies the number of states in a given energy range, near the Fermi level. Specifically, the DOS is defined as

$$D(E) = \sum_{i=1}^{2N} \int_{BZ} \delta(\Delta_i(\vec{k}) - E) d\vec{k}, \quad (59)$$

where Δ_i is the dispersion relation for the i th eigenvalue of our Hamiltonian, and we integrate over the Brillouin zone. The IDOS is defined as

$$\mu(E) = \int_0^E D(\epsilon) d\epsilon \quad (60)$$

and we only consider $E > 0$ since, in the nearest-neighbor model, we have positive and negative energy symmetry. By flatter bands, we expect higher DOS at the energy of the flat band. Moreover, a higher IDOS for low E indicates a greater number of states near the Fermi level. For DOS plots, we use Gaussian smearing with a given σ parameter to reduce numerical error, especially since the

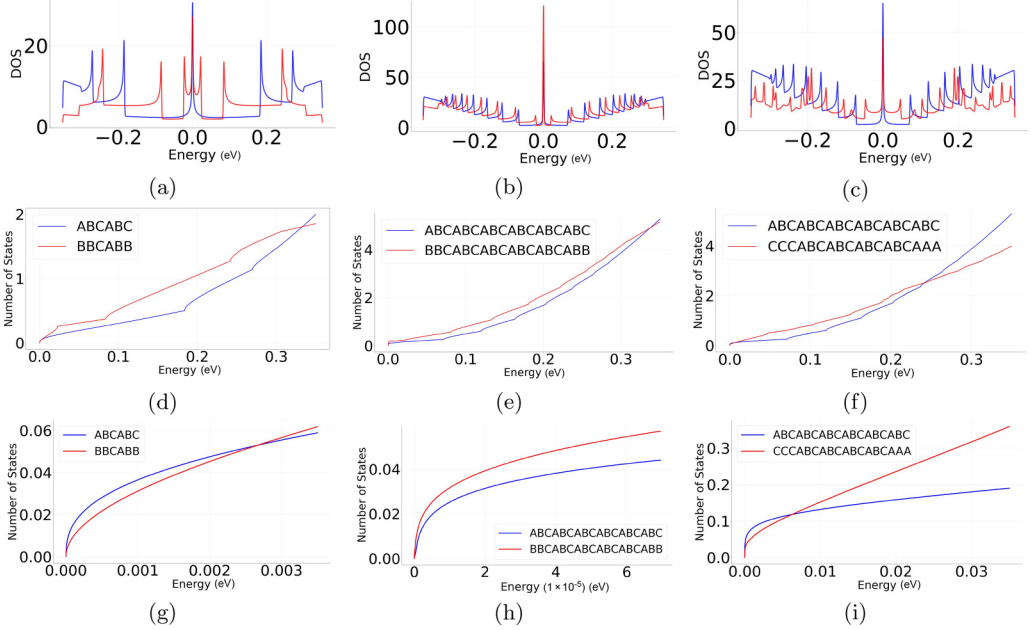


FIG. 6. Comparisons between (a)–(c) DOS calculations with Gaussian smearing $\sigma = \frac{t_1}{300}$, (d)–(f) IDOS calculations, and (g)–(i) enlarged IDOS calculations for rhombohedral stacking with parallel faults (red) and pure rhombohedral stacking (blue) with same stacking length; for panels (a), (d), and (g), $N = 6$ and we have a BB parallel fault at each end; for panels (b), (e), and (h), $N = 18$ and we have a BB parallel fault at each end; for panels (c), (f), and (i), $N = 18$ and we have a CCC parallel fault at each end. We have omitted showing specific stacking orders in the DOS plot due to lack of space, but they are shown in the IDOS plots and the colors are the same for all plots. We see that the density near the Fermi level is enhanced by adding parallel faults to the rhombohedral stacking.

DOS of a flat band is divergent. For IDOS plots, we do not apply a filter since the integrals converge. Our results are plotted in Fig. 6.

Overall, we see a viability to increase state number near the Fermi level. Not only is the zero-energy flat band enhanced in Fig. 6(b), but we also observe the shifting of external flat bands (peaks in the DOS) closer to the Fermi level in Figs. 6(a)–6(c). The IDOS within $\Delta E \approx 0.3$ of the Fermi level is higher for rhombohedral stacking with $N_i = 2$ parallel embeds, as seen in Figs. 6(d) and 6(e). Figure 6(c) shows how increasing N_i raises this difference, but lowers the energy range for which this advantage exists (for faults of length 3, $\Delta E \approx 0.25$). This shows how parallel embeds shift the states nearer to the Fermi level. We see that for small stacking length N , for example, in Figs. 6(a), 6(d), and 6(g), parallel stacking faults decrease the DOS very close to the Fermi level, as compared with pure rhombohedral stacking of the same length; this is expected since for these low stacking lengths, the change to the main flat band at the Fermi level decreases total flatness despite emergent flat bands away from the Fermi level. Increasing stacking length appears to eliminate this discrepancy. We expect that for higher stacking lengths, an addition of a single parallel fault does not greatly affect the main flat band, and therefore the flat bands outside of the Fermi level with locations independent of total stacking length, as given by Eq. (56), contribute to a net increase in DOS at and near the Fermi level.

Our derivation was done for nearest-neighbor hopping only. It is known for longer distance interactions that the dispersion relation of graphene exhibits trigonal distortions [27]. Therefore, our interpretation of rings around the K point is only valid for the region very close to the K or K' point. It is, however, still maintained that properties, such as extending the flat band, are present in

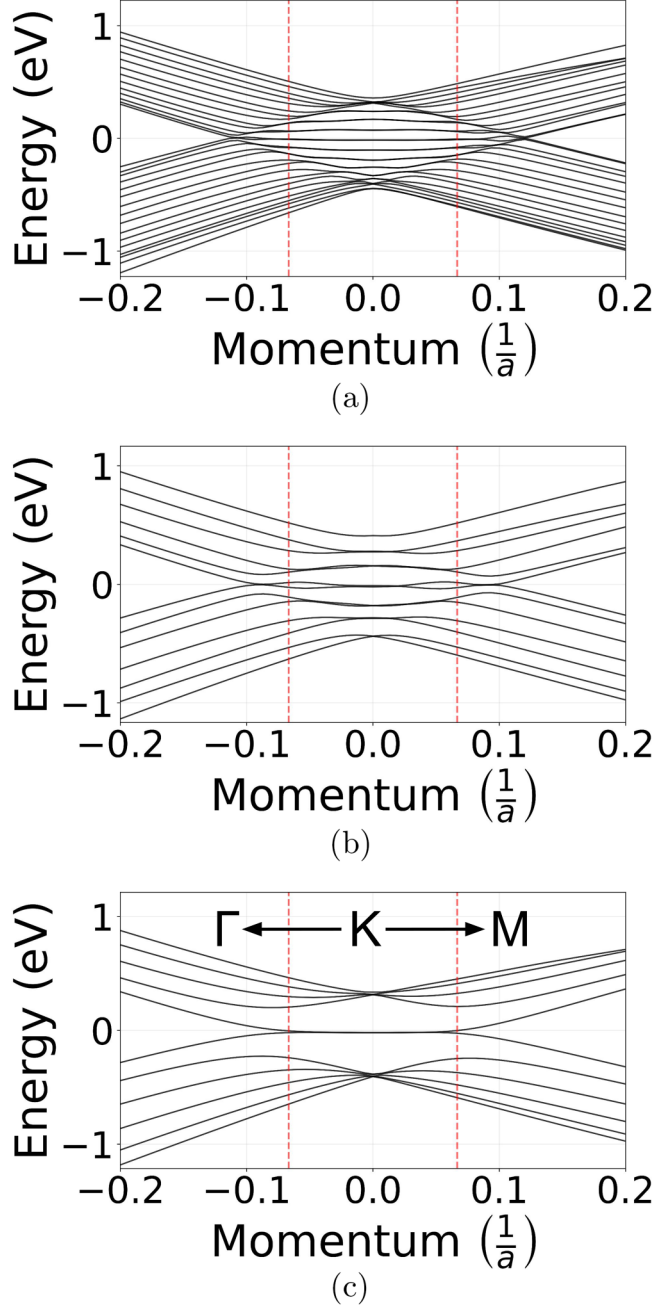


FIG. 7. DFT calculations for (a) AAAAAABCABCCCCC, (b) AAABCCC, and (c) ABCABC stackings. We have plotted our predicted rhombohedral flat band limit as given by Eq. (23) in red. Notice how panels (a) and (b) have flat bands well outside this limit. Moreover, we have plotted pure six-layer rhombohedral stacking in panel (c), including also the path in Brillouin zone, specifically setting the K point as our zero momentum, and plotting along the $\Gamma \rightarrow K \rightarrow M$ path. Note that we do not hit the Γ nor M points in our graphs because we are still focusing on momentum near K .

the dispersion relation. Moreover, the similarities between Eqs. (56) and (17) suggest the rigidity of substack properties within the whole graphene stack. To show this, we have plotted density functional theory calculations of various band structures near the K points, along the $\Gamma \rightarrow K \rightarrow M$ path as shown in the Figs. 7(a)–7(c).

For all plots, we have included the predicted ABC flat band limit (for large N) in red. In Figs. 7(a) and 7(b), we have plotted AAAAAABCABCCCCC and AAABCCC, respectively. Clearly, the flat bands of these stacking orders extend far beyond the flat band limit, as we predict by band crossings in the nearest-neighbor model. In Fig. 7(c), we have plotted ABCABC stacking for reference. We note how the flat band is much more confined to the limits provided by Eq. (23). We also note that the locations of these crossings roughly align with the nearest-neighbor model governed by Eq. (56). So, along this path, the nearest-neighbor predicted band crossings align well with more accurate calculations. We also mention that other properties of rhombohedral graphene due to long distance interactions, including broken symmetry about the Fermi level, are observed in DFT calculations, but with the same asymmetry for the flat bands at K and away from K , so that our extended flat bands maintain a similar energy level.

With our arbitrary stacking structures having shown to increase the flatness and number of states near the Fermi level, the ability to engineer a graphene stack with effective and enhanced properties from original graphene stacks with flat electronic bands is possible. The flat band of rhombohedral graphene is experimentally verified and flat bands in graphene have often been associated with interesting properties, including potential superconductivity, ferromagnetism, and strong correlation [28, 29]. Being able to extend the flat band, and in doing so increase its flatness, suggests that by incorporating stacking faults, we can produce an even flatter band than is possible with pure rhombohedral stacking only. We propose such arbitrary stackings as a powerful platform for studying flat band physics and interesting flat band properties via multilayer graphene.

IV. CONCLUSION

We have studied the electronic properties of graphene by considering the properties of the special cases of graphene stacking, AA, AB, and ABC, and applying them to a general, arbitrarily stacked multilayer graphene. We observe a remarkable level of correspondence when we incorporate these stacks together in an arbitrary fashion. Specifically, in studying stacking faults we observed that the embedding of an ABC stack could generate a flat band that very much resembles the sole ABC stack’s flat band. The possibility to induce these flat bands that generate correlated electrons while also maintaining linear bands that generate massless Dirac fermions has also been discussed. Moreover, we saw that an embedding of an AA stack allowed us to analytically solve the momenta for which there is an energy eigenvalue of zero. This then allowed us to make a more general statement about the zero-energy momenta for arbitrary stacking. The existence of these properties suggests the possibility for a more general consideration of arbitrary stacking. In general, such arbitrary stacking could contain a multitude of parallel, Bernal, and rhombohedral stacking for which one could attempt to predict the properties thereof. We have done so for the momenta for which the energy eigenvalue is zero, which we have found out is in direct relation to the existence of AA substacks; it is therefore plausible that more properties could be associated with the existence of other types of substacks. A primitive method that we have shown to be successful in many situations would be to decompose the graphene stack in a well-defined manner and considering the decomposition’s properties to then predict that of the arbitrary stack; it is qualitatively accurate for the detection of flat bands and quantitatively accurate for finding the rings of zero energy. These calculations furthermore show the ability to extend the flat band of graphene, which is promising for enhancing its many notable properties.

DATA AVAILABILITY

The data that support the findings of this article are not publicly available. The data are available from the authors upon reasonable request.

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