Evolution and dimensional crossover from the bulk subbands in ABC-stacked graphene to a three-dimensional Dirac cone structure in rhombohedral graphite

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(Dated: July 6, 2015)

Abstract

The band structure of ABC-stacked $N$-layer graphene comprises topologically corresponding flat surface and gapped bulk subbands, as a consequence of the unique stacking configuration. In this paper, the bulk subbands are for the first times ever obtained for arbitrary $N$. A non-perturbative effective Hamiltonian closed in the bulk subspace is derived and used. The gapped bulk subbands are shown to evolve towards the zero energy with increasing $N$ and in the infinite limit, they touch linearly along a circle. This outcome is a manifestation of the dimensional crossover to a three-dimensional Dirac cone structure known to exist in the bulk of rhombohedral graphite. The Dirac points, forming continuous nodal lines in a spiraling fashion, are projected onto the circle, within which the surface subbands are confined and flatten.

PACS numbers: 71.20.-b, 73.21.Ac, 73.22.Pr
I. INTRODUCTION

The symmetrical and topological properties of graphene layers and their stacks have opened up new fields of physical research in the past decade. According to the hexagonal lattice symmetry, a number of graphene layers can be so stacked that any adjacent two are shifted from each other in either direction along the armchair orientation. Among others, ABC-stacking configuration is especially noticeable in that all the layers are shifted in a unique direction. A non-trivial topological phase is accommodated therein, giving rise to surface states that are localized at the outermost layers and coupled to the rest, so-called bulk states. This is distinct from AB-stacking configuration, whose trivial topology does not render any surface states. In general, these surface states are characterized by flat band dispersion about the zero energy. It is well known that the flat surface subbands in ABC-stacked \( N \)-layer graphene can be obtained from a chiral effective Hamiltonian with chirality \( J = N \). Corresponding quantum Hall effects (QHEs) have been predicted and observed at least for \( N = 3 \). Apart from the surface subbands, the bulk subbands are gapped and seem to be intricate. They evolve to be even more complex with increasing \( N \) while the surface subbands are more and more flat. So far, the bulk subbands remain unsolved, probably because no attractive properties are expected from them. There is, however, something remarkable in their evolution to the three-dimensional (3D) realm as is highlighted in recent research.

In the 3D counterpart of ABC-stacked \( N \)-layer graphene, namely, rhombohedral graphite (RG), the bulk atomic lattice is usually modelled by infinitely many layers. There is a crossover of lattice symmetry when \( N \) goes from being finite to being infinite, with a two-atom rhombohedral lattice appearing in RG. The resulting \( 2 \times 2 \) chiral Hamiltonian leads to a 3D Dirac cone structure, where the Dirac points (DPs) form continuous lines in a spiraling fashion in association with a sausage-like Fermi surface. Such gapless bulk subbands in RG can be used to explain the 3D QHE observed in graphite, in which the transport takes place in each layer with \( J = 1 \) charge carriers and the quantization of the conductivity is the same as in monolayer graphene. This is a general attribute of graphite as a weakly coupled layered system. The interlayer hopping brings about the described 3D features of the bulk subbands in RG, whereas its much smaller ratio to the intralayer hopping is also responsible for the 2D transport character revealed in the 3D QHE. Indeed,
the dimensionality of graphite can be effectively determined by the interplay between the
interlayer hopping and the interlayer Coulomb interaction, the latter being absent from
the single-particle Hamiltonian. In this regard, the 3D nature of the Dirac cone structure in
RG has been verified by the existence of optical magnetoplasmons in the presence of that
interplay.

The non-trivial topology uniquely endowed in the ABC stack of graphene layers leads to
a bulk-surface correspondence in RG, just as the bulk-edge correspondence in monolayer
graphene with zigzag edges. The topological stability against perturbative disturbance
such as impurities and crystal deformations is ensured by the DP spirals, which are nodal
lines just as the DPs are nodal points in monolayer graphene. Consequently, RG possesses
metallic flat surface subbands while being semimetallic in the bulk with a 3D Dirac cone
structure. As such, RG can be compared to certain topological insulators, e.g., Bi$_2$Se$_3$ and
Bi$_2$Te$_3$, which are also ABC-stacked layered materials.

Since the physics arising from ABC-stacking configuration is so rich and deep, it is of
interest to investigate the band structure of ABC-stacked $N$-layer graphene ranging from
2D to 3D realm. Recently, first-principle calculations simultaneously taking into account
the surface and the bulk states have been performed with a number of layers up to $N = 10$,showing that the bulk subbands are still gapped. A recursive analysis has been achieved
for infinite $N$ and the resulting density of states (DOS) and Landau level spectrum are
the same as in monolayer graphene in agreement with the 3D Dirac cone structure. It is
therefore reasonable to envisage a dimensional crossover from the gapped bulk subbands to
the 3D Dirac cone structure. Nevertheless, to our knowledge the evolution has not been
ever explicitly studied in spite that similar studies of AB stacks have been conducted.

In this paper, we analytically calculate the bulk subbands in ABC-stacked $N$-layer
graphene by deriving and using an expression for arbitrary $N$. We investigate their evolu-
tion in the increase of $N$ and dimensional crossover in the infinite limit of $N$. In Sec. II
we describe the model and construct a 2D non-perturbative effective Hamiltonian closed in
the bulk subspace so as to treat the coupling to the surface subbands. The obtained bulk
subbands are certain 2D projections from the 3D Dirac cone structure in RG. In Sec. III, we
describe how to resolve a second-order recursion involved in the eigenvalue problem of the
effective Hamiltonian. Then we derive the expression of the eigenenergies and bulk DOS.
In Sec. IV, at first we analyze the bulk subbands and demonstrate their evolution together
with the well understood surface subbands. Then we elucidate the dimensional crossover. Finally, we give in Sec. V a summary with an outlook.

II. MODEL AND THE EFFECTIVE HAMILTONIAN

The lattice of ABC-stacked $N$-layer graphene is schematically shown in Fig. 1(a), where graphene layers infinitely extended in the $(x,y)$ plane and stacked along the $z$ direction are labeled by $1, 2, \ldots, N$, with the lattice constant of a single layer $a = 0.246$ nm and interlayer distance $d = 0.337$ nm. Carbon atoms in this configuration are classified into two sets. One set contains the sublattices of surface atoms ($B_1$ and $A_N$); the other contains the sublattices of the bulk atoms. Each bulk atom is vertically bonded with another one that is located in either the adjacent upper or the adjacent lower layer. In the two outermost layers the surface atoms are free from such bonding. A solid view in Fig. 1(b) illustrates that infinitely many ABC-stacked graphene layers are taken to model the bulk of RG, which has a two-atom rhombohedral primitive unit cell. Also shown in Fig. 1(b), for reference, is an alternatively set hexagonal non-primitive unit cell of triple volume, which is also the primitive unit cell in ABC-stacked trilayer graphene.

From ABC-stacked graphene\textsuperscript{22-24} to RG\textsuperscript{25} there always exist coupled surface and bulk subbands, respectively localized at the surface and the bulk atomic sublattices. The conventional tight-binding (TB) model is set forth in Fig. 1(a),\textsuperscript{13,26,27} where those nearest-neighbor electron hoppings are shown. The bulk subbands have been known to correspond to the 2D projection of a DP spiral surrounds the $K(\prime)$ point of the 2D hexagonal Brillouin zone (BZ)\textsuperscript{211} as shown in Fig. 1(c). The projection is close to the annular valleys that are present in the bulk subbands in ABC-stacked graphene\textsuperscript{12,24} A 3D rhombohedral-to-2D hexagonal zone-folding relation could be in principle figured out to obtain the 2D bulk subbands. However, one cannot do a straight folding along the stacking direction ($k_z$) here as one does for AB-stacked graphite.\textsuperscript{29} This fact can be understood since the vertical line through $K(\prime)$ is no longer a symmetry line in the 3D rhombohedral BZ.\textsuperscript{11,11} We shall derive a 2D effective Hamiltonian in the bulk subspace, which is used together with the well realized effective Hamiltonian in the surface subspace.\textsuperscript{6,7} The evolution and dimensional crossover can be clarified once the eigenenergies are solved out for arbitrary $N$. Such methodology using
subspace effective Hamiltonians has been applied to study AB-stacked $N$-layer graphene, for which the subband indices are directly related to the projections of the 3D band structure at allowed $k_z$, in consistency with the vertical zone-folding scheme. Although a direct relation between the bulk subband index and $k_z$ is not accessible for ABC-stacked $N$-layer graphene, it is rational to relate the indices to certain 2D projections from the 3D Dirac cone structure at all allowed $\mathbf{k} = (k_x, k_y, k_z)$ in the 3D rhombohedral BZ. The hexagonal BZ of the stack of $N$ layers becomes extremely thinned as $N$ goes infinitely large, so that we have an approximately zero extent in the $k_z$ dimension. Hence, the continuum of projections forming a bulk zone in the 2D hexagonal BZ is acquired.

The model is described as follows. Referring to Fig. 1(a), the nearest interlayer hopping, $\beta_1$, takes place between the vertically bonded bulk atoms in adjacent layers. Those interlayer hoppings other than $\beta_1$ alter the surface subbands but they only perturb the bulk subbands. The minimal model including only $\beta_1(= 0.32$ eV) and the nearest intralayer hopping $\beta_0(= -2.73$ eV) suffices for our purpose. The Hamiltonian $\mathcal{H}^{(N)}$, based on the TB Bloch functions $(\phi_{B_1}, \phi_{A_N}, \phi_{A_1}, \phi_{B_2}, \phi_{A_2}, \phi_{B_3}, \ldots, \phi_{A_{N-1}}, \phi_{B_N})$ with respect to the $2N \times 2N$ sublattices, is represented as

$$
\mathcal{H}^{(N)} = 
\begin{pmatrix}
0 & 0 & v\pi^\dagger & 0 & 0 & 0 & 0 & \ldots & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 & 0 & 0 & 0 \\
v\pi & 0 & 0 & \beta_1 & 0 & 0 & 0 & \ldots & 0 & 0 & 0 & 0 \\
0 & 0 & \beta_1 & 0 & v\pi^\dagger & 0 & 0 & \ldots & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & v\pi & 0 & \beta_1 & 0 & \ldots & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \beta_1 & 0 & v\pi^\dagger & \ldots & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & v\pi & 0 & \ldots & 0 & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 & \beta_1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \ldots & \beta_1 & 0 & v\pi^\dagger & 0 \\
v\pi^\dagger & 0 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 & \beta_1 & 0 & 0 \\
v\pi^\dagger & 0 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 & \beta_1 & 0 & 0 \\
\end{pmatrix}_{2N \times 2N},
$$

with $v = (\sqrt{3}/2)a\beta_0/h$ and $\pi = \xi p_x + ip_y$, where $(p_x, p_y)$ is the momentum measured from $K^{(i)}$ and $\xi = \pm 1$ are the valley index for $K$ and $K'$, respectively. The two DP spirals with respect to $K$ and $K'$ have clockwise and counterclockwise spiraling senses with increasing
k_z^{11}$ as shown in Fig. 1(c). Without loss of generality, we take $\xi = 1$ for $K$ below. It is noted that within the minimal model, the DP spiral is laid on a cylinder surface around the vertical line through $K^{(r)}$ and therefore its 2D projection becomes a circle around $K^{(r)}$. For the scale of $(p_x^2 + p_y^2)^{1/2} = p$, we remark the radius of the projected DP spiral $p_D = \frac{\beta_1}{v}$.

This delimits the boundary of the non-trivial topology for the bulk-surface correspondence.

The Hamiltonian $H^{(N)}$ in Eq. (1) is partitioned as follows. The upper left $2 \times 2$ block is denoted by $H^{(N)}_{11}$ with respect to the surface subspace spanned by $(\phi_B, \phi_A)$, and the lower right $(2N - 2) \times (2N - 2)$ block is $H^{(N)}_{22}$ for the bulk subspace spanned by the bulk sublattices. The coupling between $H^{(N)}_{11}$ and $H^{(N)}_{22}$ is given by the off-diagonal blocks $H^{(N)}_{12}$ and $H^{(N)}_{21}$ $[= (H^{(N)}_{12})^\dagger]$. It is easy to identify the surface subbands as being lower in energy than the bulk subbands. The secular equation reduces to $\det (H^{(N)} - \varepsilon) = \varepsilon^2 (\varepsilon^2 - \beta_1^2)^{N-1} = 0$ at $K$, where the coupling is absent since $H^{(N)}_{12}$ and $H^{(N)}_{21}$ are zero matrices with $\pi = 0$. The lowest eigenenergy $\varepsilon = 0$ is associated with two degenerate eigenstates in the surface subspace, while the eigenenergies $\varepsilon = \pm \beta_1$ are each associated with $N - 1$ degenerate eigenstates in the bulk subspace. Our goal is to construct an effective Hamiltonian in the bulk subspace and solve the eigenvalues for arbitrary $N$. That is, a block diagonalization for the full Hamiltonian $H^{(N)}$ is required:

$$H^{(N)} = \begin{pmatrix} H^{(N)}_{\text{surf}} & 0 \\ 0 & H^{(N)}_{\text{bulk}} \end{pmatrix},$$

where $H^{(N)}_{\text{surf}}$ and $H^{(N)}_{\text{bulk}}$ are the effective Hamiltonians in the surface and the bulk subspaces, respectively. Considering the full Hamiltonian [see Eq. (1)] with $\pi \neq 0$ in general, we expand its eigenvectors as $|\psi_n\rangle = \sum_{m=1}^{2N} C_{mn} |\psi_m^{(0)}\rangle$ in terms of the eigenvectors $|\psi_m^{(0)}\rangle$ of the uncoupled Hamiltonian ($\pi = 0$). Hence, the Schrödinger equation is reformulated to be

$$\begin{pmatrix} H^{(N)}_{11} - \varepsilon & H^{(N)}_{12} \\ H^{(N)}_{21} & H^{(N)}_{22} - \varepsilon \end{pmatrix} \begin{pmatrix} C_1 \\ C_2 \end{pmatrix} = 0,$$

where $C_1$ and $C_2$ are, respectively, $2 \times 2N$ and $(2N - 2) \times 2N$ partitions of the coefficient matrix $(C_{mn})$. The block diagonalization in Eq. (3) is then conceptually performed by a similarity transformation of the basis from the set of $\{|\psi_m^{(0)}\rangle\}$ to the unsolved set of $\{|\psi_n\rangle\}$.
From Eq. (4) the effective Hamiltonian \(H_{\text{surf}}^{(N)}\) in the surface subspace is given by

\[
H_{\text{surf}}^{(N)}(\varepsilon) = H_{11}^{(N)} - H_{12}^{(N)} (H_{22}^{(N)} - \varepsilon)^{-1} H_{21}^{(N)},
\]

and the effective Hamiltonian \(H_{\text{bulk}}^{(N)}\) in the bulk subspace is

\[
H_{\text{bulk}}^{(N)}(\varepsilon) = H_{22}^{(N)} - H_{21}^{(N)} (H_{11}^{(N)} - \varepsilon)^{-1} H_{12}^{(N)}.
\]

The derivation of Eq.s (5) and (6) for the effective Hamiltonians is consistent with the use of the Green’s function \(G^{(N)}(\varepsilon) = (\mathcal{H}^{(N)} - \varepsilon)^{-1}\) such that we have \(G_{11/22}^{(N)}(\varepsilon) = (H_{\text{surf/bulk}}^{(N)} - \varepsilon)^{-1}\), for which the partitions \(G_{11}^{(N)}\) and \(G_{22}^{(N)}\) of the Green’s function \(G^{(N)}\) can be explicitly obtained.\(^{30}\)

The effective Hamiltonians shown in Eq.s (5) and (6) depend on the energy \(\varepsilon\) due to the coupling between the surface and the bulk subbands. This might be deemed the price for the reduction in dimension. An effective Hamiltonian can even be non-Hermitian in general, but this is not the case here. At first sight, a perturbation calculation is expected as usual. Unfortunately, divergence of the perturbation series would be encountered if the coupling is strong compared with a diminishing bulk energy gap as envisaged here for infinitely large \(N\). We shall take a non-perturbative approach below, which is accessible owing to the specific form of Eq.s (5) and (6). It is noted that the similarity transformation for the block diagonalization is not unique in general, while different effective Hamiltonians obtained through different transformations yield the same eigenvalues.

The surface subbands have been well realized by the chiral effective Hamiltonian \(H_{\text{chiral}}^{(3)}\) for ABC-stacked trilayer graphene.\(^{7,8}\) This can be obtained in the present framework by removing the \(\varepsilon\)-dependence due to the powers of \(\varepsilon/|H_{22}^{(N)}|\) in the coupling term of \(H_{\text{surf}}^{(N)}\) in Eq. (5). The chiral effective Hamiltonian for arbitrary \(N\) can be deduced to be\(^6\)

\[
H_{\text{chiral}}^{(N)} = (-\frac{1}{\beta_1})^{N-1} \begin{pmatrix} 0 & (v\pi)^N \\ (v\pi)^N & 0 \end{pmatrix}.
\]

It should be noted that the use of \(H_{\text{chiral}}^{(N)}\) fails outside the interval between the \(K\) point and the projection of the DP spiral, \(0 < p < p_D = \beta_1/v\), because it is derived by the power expansion of \(\varepsilon/|H_{22}^{(N)}|\)(\(\ll 1\)). Inside the interval, the surface subbands are more and more flat and approach the zero energy.\(^{31}\)

The effective Hamiltonian \(H_{\text{bulk}}^{(N)}(\varepsilon)\) in the bulk space is deduced from Eq. (6) without any perturbation or power expansion. The effect of the surface on the bulk subbands are thus
completely retained. In so doing we can reach the region around \( p = p_D \), onto which the DP spiral is projected, even though the energy gap is known to be nearly closed up for infinitely large \( N \). Because \( H_{11}^{(N)} \) is zero in Eq. (1), the coupling term \(-H_{21}^{(N)}(H_{11}^{(N)} - \varepsilon)^{-1}H_{12}^{(N)}\) in Eq. (6) has non-vanishing elements at the two diagonal corners only, given by \((vp)^2/\varepsilon\). Therefore, the coupling is almost absent from the vicinity of \( K \) with \( p \approx 0 \) and \( \varepsilon \approx \beta_1 \gg 0 \), where the effective Hamiltonian is identical to the block with respect to the bulk subspace:

\[
H_{\text{bulk}}^{(N)}(\varepsilon \to \beta_1) = H_{22}^{(N)}. \tag{8}
\]

In general, the non-perturbative effective Hamiltonian \( H_{\text{bulk}}^{(N)}(\varepsilon) \) is given by

\[
H_{\text{bulk}}^{(N)}(\varepsilon) = \begin{pmatrix}
(vp)^2\varepsilon^{-1} & \beta_1 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\
\beta_1 & 0 & v\pi^\dagger & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\
0 & v\pi & 0 & \beta_1 & 0 & \cdots & 0 & 0 & 0 & 0 \\
0 & 0 & \beta_1 & 0 & v\pi^\dagger & \cdots & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & v\pi & 0 & \cdots & 0 & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \cdots & 0 & \beta_1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \cdots & \beta_1 & 0 & v\pi^\dagger & 0 \\
0 & 0 & 0 & 0 & 0 & \cdots & 0 & v\pi & 0 & \beta_1 \\
0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & \beta_1 & (vp)^2\varepsilon^{-1}
\end{pmatrix}_{(2N-2)\times(2N-2)}. \tag{9}
\]

In comparison with Eq. (7) for \( H_{\text{surf}}^{(N)} \), where the effect of the bulk subbands on the surface subbands is significant, Eq. (9) shows that the coupling effect on the bulk subbands is relatively weak. It is observed that \( H_{\text{bulk}}^{(N)}(\varepsilon) \) has a nested structure as well as \( H_{22}^{(N)} \) does, a characteristic of ABC-stacking configuration.

### III. BULK SUBBANDS IN ABC-STACKED \( N \)-LAYER GRAPHENE

#### A. Resolution for the secular equation

For the bulk subbands in ABC-stacked \( N \)-layer graphene, the eigenenergies of the effective Hamiltonian \( H_{\text{bulk}}^{(N)}(\varepsilon) \) described in Eq. (9) are solved from the secular equation \( \det (H_{\text{bulk}}^{(N)}(\varepsilon) - \varepsilon) = 0 \). Owing to the nested structure of \( H_{\text{bulk}}^{(N)}(\varepsilon) \), a second-order recursion
is involved. The secular equation is separated as

\[ \det \left( H_{\text{bulk}}^{(N)}(\varepsilon) - \varepsilon \right) \overset{\text{def}}{=} f_N(\varepsilon) + \frac{(vp)^2}{\varepsilon} g_{N-1}(\varepsilon) = 0, \]  

(10)

where \( f_N(\varepsilon)[= \det (H_{22}^{(N)} - \varepsilon)] \) and \( g_{N-1}(\varepsilon) \) are given by

\[
f_N(\varepsilon) = \det \begin{pmatrix}
-\varepsilon & \beta_1 & 0 & 0 & 0 & \ldots & 0 & 0 & 0 & 0 \\
\beta_1 & -\varepsilon & v\pi^\dagger & 0 & 0 & \ldots & 0 & 0 & 0 & 0 \\
0 & v\pi & -\varepsilon & \beta_1 & 0 & \ldots & 0 & 0 & 0 & 0 \\
0 & 0 & \beta_1 & -\varepsilon & v\pi^\dagger & \ldots & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & v\pi & -\varepsilon & \ldots & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & 0 & 0 & \ldots & -\varepsilon & \beta_1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \ldots & \beta_1 & -\varepsilon & v\pi^\dagger & 0 \\
0 & 0 & 0 & 0 & 0 & \ldots & \beta_1 & -\varepsilon & \beta_1 & 0 \\
0 & 0 & 0 & 0 & 0 & \ldots & 0 & 0 & \beta_1 & -\varepsilon \\
\end{pmatrix}_{(2N-2)\times(2N-2)} \]

(11)

\[
g_{N-1}(\varepsilon) = \det \begin{pmatrix}
-\varepsilon & v\pi^\dagger & 0 & \ldots & 0 & 0 & 0 \\
v\pi & -\varepsilon & \beta_1 & \ldots & 0 & 0 & 0 \\
0 & \beta_1 & -\varepsilon & \ldots & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & \ldots & -\varepsilon & v\pi^\dagger & 0 \\
0 & 0 & 0 & \ldots & v\pi & -\varepsilon & \beta_1 \\
0 & 0 & 0 & \ldots & 0 & \beta_1 & -\varepsilon \\
\end{pmatrix}_{(2N-3)\times(2N-3)} \]

(12)

Note that \( g_{N-1}(\varepsilon) \) comes from the coupling to the surface subbands. The nested structure in Eqs (11) and (12) brings about

\[
f_N(\varepsilon) = -\beta_1^2 f_{N-1}(\varepsilon) - \varepsilon g_{N-1}(\varepsilon), \]

\[
g_{N-1}(\varepsilon) = -\varepsilon f_{N-1}(\varepsilon) - (vp)^2 g_{N-2}(\varepsilon), \quad N \geq 3, \]

(13)

which reduces to a second-order recursive equation

\[
f_N(\varepsilon) = (r + s) f_{N-1}(\varepsilon) - rs f_{N-2}(\varepsilon), \quad N \geq 3, \]

(14)

where

\[
r + s = \varepsilon^2 - \beta_1^2 - (vp)^2, \quad rs = \beta_1^2 (vp)^2. \]

(15)
From Eq. (11), the initial conditions are given by

\[ f_1(\varepsilon) = 1, \quad f_2(\varepsilon) = \varepsilon^2 - \beta_1^2 - (vp)^2. \] (16)

The recursion for \( g_{N-1}(\varepsilon) \) has the same form as for \( f_N(\varepsilon) \) in Eq. (14), with more tedious initial conditions.

We rewrite Eq. (14) as

\[ f_N(\varepsilon) - rf_{N-1}(\varepsilon) = s(f_{N-1}(\varepsilon) - rf_{N-2}(\varepsilon)) \]

in order to resolve \( f_N(\varepsilon) \) with the initial conditions given in Eq. (16) by two steps. At first, we get

\[ f_N(\varepsilon) - rf_{N-1}(\varepsilon) = s^{N-2}(f_2(\varepsilon) - rf_1(\varepsilon)). \]

Then we achieve the resolution and express \( f_N(\varepsilon) = r^{N-1}f_1(\varepsilon) + \sum_{\nu=2}^{N} r^{N-\nu}s^{\nu-2}(f_2(\varepsilon) - rf_1(\varepsilon)) \) for arbitrary \( N \). A concise form of resolved \( f_N(\varepsilon) \) is written as

\[ f_N(\varepsilon) = \frac{1}{r-s][(r^{N-1} - s^{N-1})f_2(\varepsilon) - rs(r^{N-2} - s^{N-2})f_1(\varepsilon)], \quad N \geq 3. \] (17)

With Eq. (17), the resolved expression of \( g_{N-1}(\varepsilon) \) can be obtained from Eq.s (13).

B. Eigenenergy spectrum

In proceeding to solve the eigenvalue problem of \( H^{(N)}_{\text{bulk}}(\varepsilon) \) from Eq. (10), now the resolved terms \( f_N(\varepsilon) \) and \( g_{N-1}(\varepsilon) \) obtained from Eq.s (13) and (17) are manipulated further. The variables \( r \) and \( s \) defined in Eq. (15) form a complex conjugate pair if

\[ (r+s)^2 - 4rs = [\varepsilon - (\beta_1 + vp)][\varepsilon - (\beta_1 - vp)][\varepsilon + (\beta_1 + vp)][\varepsilon + (\beta_1 - vp)] < 0. \] (18)

We take Eq. (18) as a priori true, which leads to self-consistent results as shown in the following. Thus, all the eigenvalues are definitely enveloped by the branches \( \varepsilon - (\beta_1 \pm vp) = 0 \) and \( \varepsilon + (\beta_1 \pm vp) = 0 \).

By changing variables as \( r = \eta e^{i\theta} \) and \( s = \eta e^{-i\theta} \), Eq. (15) is equivalent to

\[ \eta = \beta_1 vp, \quad \cos \theta = \frac{\varepsilon^2 - \beta_1^2 - (vp)^2}{2\beta_1 vp}, \] (19)

which provides an easy-to-handle connection between the eigenvalue \( \varepsilon \) and variable \( \theta \). Accordingly, Eq. (17) is transformed to be

\[ f_N(\varepsilon) = \frac{\eta^{N-1}}{\sin \theta} \sin N\theta, \quad N \geq 3, \] (20)
with the aid of the trigonometric identity \(2 \cos \theta \sin (N - 1)\theta - \sin (N - 2)\theta = \sin N\theta\). Using Eq.s (13) With Eq. (17) again, we also have

\[
g_{N-1}(\varepsilon) = -\frac{\beta_1 \eta^{N-2}}{\varepsilon \sin \theta} (v_p \sin N\theta + \beta_1 \sin (N-1)\theta), \quad N \geq 3. \tag{21}
\]

Consequently, the secular Eq. (10) is transformed to be

\[
\frac{\beta_1^2 \eta^{N-1}}{\varepsilon^2 \sin \theta} (\sin N\theta + \frac{v_p}{\beta_1} \sin (N+1)\theta) = 0, \quad N \geq 3, \tag{22}
\]

where Eq. (19) is used. There are \(N - 1\) roots to Eq. (22) in correspondence to the \(2N - 2\) eigenvalues of \(H_{\text{bulk}}^{(N)}(\varepsilon)\). Once those roots \(\theta_j(p), j = 1, 2, \ldots, N - 1\), as functions of \(p\) are determined, the whole eigenenergy spectrum of \(H_{\text{bulk}}^{(N)}(\varepsilon)\) can be acquired according to Eq. (19). That is,

\[
\pm \varepsilon_j(p) = \pm [\beta_1^2 + (v_p)^2 + 2\beta_1 v_p \cos \theta_j(p)]^{1/2}, \quad j = 1, 2, \ldots, N - 1, \tag{23}
\]

where \(j\) is the subband index and \(\pm\) denote, respectively, the conduction and the valence bulk subbands. The quantum number \(j\) is related to the allowed 2D projections from the 3D Dirac cone structure.

To find out \(\theta_j(p)\) we firstly survey the region where the term \(v_p/\beta_1\) in Eq. (22) can be approximately dropped. Then we go away from \(v_p/\beta_1 = 0\) at \(K\) and reach \(v_p/\beta_1 \approx 1\) around the 2D projection \(p D\) of the DP spiral [see Eq. (2)]. With \(v_p/\beta_1 = 0\), the roots \(\theta_j(p)\) are simply specified by \(\sin N\theta = 0, N \geq 3\), given by

\[
\theta_j = j\pi/N, \quad j = 1, 2, \ldots, N - 1. \tag{24}
\]

With \(v_p/\beta_1 = 1\), Eq. (22) becomes \((\beta_1^2 \eta^{N-1}/2\varepsilon^2 \sin (\theta/2)) \sin (N+1/2)\theta = 0, N \geq 3\). For \(\sin (N+1/2)\theta = 0\), the roots \(\theta_j(p)\) are given by

\[
\theta_j = \frac{j\pi}{N + \frac{1}{2}}, \quad j = 1, 2, \ldots, N - 1. \tag{25}
\]

In Eq.s (24) and (25), the numerals \(j\) are so specified as to exclude the case of \(\sin \theta = 0\) and to omit double counting of the value of \(\cos \theta\). The two sets of \(\theta_j\) at the two ends of \(v_p/\beta_1\) are somewhat different, but with increasing \(N\) they approach and ultimately coincide with each other. Between the two ends, we directly calculate \(\theta_j(p)\) from Eq. (22) for few-layer graphene. For large \(N\), the use of either Eq. (24) or Eq. (25) is convenient.
C. Bulk density of states

It is conventionally known that the local DOS in a space is related to a Green’s function. We firstly establish this relationship in the bulk subspace. If \( \varepsilon \rightarrow \varepsilon + i0^+ \) is made, the related Green’s function reads

\[
G_{22}^{(N)}(\varepsilon + i0^+) = (H_{\text{bulk}}^{(N)}(\varepsilon) - \varepsilon - i0^+)^{-1}.
\]

Referring to Eq. (23), the subband index \( j(= 1, 2, \ldots, N - 1) \) and band index \( \mu(= \pm) \) are lumped as \( \lambda = (j, \mu) \) in the following. In the eigenspace of \( H_{\text{bulk}}^{(N)}(\varepsilon) \), where the eigenvector and eigenvalue are respectively denoted by \( |\psi_\lambda\rangle \) and \( \varepsilon_\lambda \), the Green’s function represented as \( \sum_\lambda |\psi_\lambda\rangle \langle \psi_\lambda| (H_{\text{bulk}}^{(N)}(\varepsilon) - \varepsilon - i0^+)^{-1} |\psi_\lambda\rangle \langle \psi_\lambda| \) reduces to

\[
G_{22}^{(N)}(\varepsilon + i0^+) = - \sum_\lambda \frac{|\langle \psi_\lambda| \psi_\lambda \rangle|}{\varepsilon - \varepsilon_\lambda + i0^+},
\]

for which the identity \( \langle \psi_\lambda| O| \psi_\lambda \rangle^{-1} = \langle \psi_\lambda| O^{-1}| \psi_\lambda \rangle \) for an operator \( O \) is used. Based on the \( 2N - 2 \) TB Bloch functions \( |\phi_l\rangle \), the imaginary part of the diagonal element \( g_{ll} \) of \( G_{22}^{(N)}(\varepsilon + i0^+) \) in Eq. (26) is given by

\[
\text{Im} \ g_{ll} = \pi \sum_\lambda |c_M|^2 \delta(\varepsilon - \varepsilon_\lambda), \quad l = 1, 2, \ldots, 2N - 2,
\]

with \( c_M = \langle \phi_l| \psi_\lambda \rangle \) being the component of \( |\psi_\lambda\rangle \) at the \( l \)th bulk sublattice, where \( \pi \delta(t) = u/(t^2 + u^2) \), \( u \rightarrow 0 \), is defined for the delta function. The local DOS has a manifestation in Eq. (27) since the eigenvector \( |\psi_\lambda\rangle \) contributes a probability density \( |c_M|^2 \) at the \( l \)th bulk sublattice. In the infinitely extended \((x, y)\) plane, the number of states is obtained by counting the allowed wave vectors \( k_\| = (k_x, k_y) \). Hence, the local DOS is given by

\[
D_{ll}^{(N)}(\varepsilon) = \frac{1}{\pi} \int_{BZ} \frac{dk_\|}{(2\pi)^2} \text{Im} \ g_{ll},
\]

where the integration turns out to run along the circular isoenergetic path with respect to each subband \( \varepsilon_\lambda(p = \hbar k) \) given in Eq. (23).

Since all the bulk atoms are indistinguishable in the infinite limit of \( N \), we are going to calculate the bulk DOS for arbitrary \( N \) and observe the evolution. The bulk DOS is obtained from the local DOS in Eq. (28) by summing \( D_{ll}^{(N)}(\varepsilon) \) over all the \( 2N - 2 \) bulk sublattices and is thus given by \( D_{\text{bulk}}^{(N)}(\varepsilon) = \sum_{l=1}^{2N-2} D_{ll}^{(N)}(\varepsilon) \). This leads to

\[
D_{\text{bulk}}^{(N)}(\varepsilon) = \sum_\lambda \int_{BZ} \frac{dk}{(2\pi)^2} \delta(\varepsilon - \varepsilon_\lambda(k)),
\]
where $\sum_{l}^{2N-2} |c_{\lambda}|^2 = 1$ for normalized $|\psi_{\lambda}\rangle$. Note that the superscript $N$ of $D_{\text{bulk}}^{(N)}(\varepsilon)$ is implied by the up bound of $j$ in $\lambda$. In performing the calculation with Eq. (29), we use the Lorentzian $(\Gamma/\pi)[(\varepsilon - \varepsilon_{\lambda}(k))^2 + \Gamma^2]^{-1}$ with a tiny width $\Gamma$ to approximate the delta function $\delta(\varepsilon - \varepsilon_{\lambda}(k))$.

IV. RESULTS AND DISCUSSION

A. Evolution

The eigenenergies $\pm \varepsilon_j(p)$ of $H_{\text{bulk}}^{(N)}(\varepsilon)$ for the bulk subbands are calculated from Eq. (23) for various numbers ($N$) of ABC-stacked graphene layers. The results are presented and discussed below, together with the energies of the surface subbands

$$\frac{\varepsilon}{\beta_1} = \pm \left(\frac{vp}{\beta_1}\right)^N,$$

which is obtained from the chiral effective Hamiltonian $H_{\text{chiral}}^{(N)}$ given in Eq. (7). In Fig. 2, the evolution of the band structure of ABC-stacked graphene is clear in an overview from a few layers ($N = 3, 4, \ldots, 8$) to a lot of layers ($N \approx 100$). Certainly, the surface subbands are rapidly flatten inside the interval $0 < vp/\beta_1 < 1 = vp_{D}/\beta_1$. It is noted that the use of $H_{\text{chiral}}^{(N)}$ fails dramatically outside this interval, whereas actually the surface subbands should be suppressed due to band repulsion. This failure can be circumvented using the full Hamiltonian consisting of coupled surface and bulk states, whether around the $K$ point or over the whole BZ. By contrast, our results from the non-perturbative $H_{\text{bulk}}^{(N)}(\varepsilon)$ for the bulk subbands agree with those obtained using the full Hamiltonian over a wide region.

The intricate bulk subbands can be unraveled by analyzing the expression of $\pm \varepsilon_j(p)$ given in Eq. (23). Obviously, the eigenenergy spectrum has isotropic and electron-hole symmetries, as a consequence of the minimal model. All the $N-1$ conduction bulk subbands $\varepsilon_j(p)$, as well as all the $N-1$ valence bulk subbands $-\varepsilon_j(p)$, are degenerate at the $K$ point. To be explicit, those $\theta_j$ given in Eq. (24), which is derived about $K$, are paired according to $\cos \left(\frac{j\pi}{N}\right) = -\cos \left(\frac{(N-j)\pi}{N}\right)$; in particular, $\cos \theta_{N/2} = 0$ stands solely if $N$ is even. Therefore, near $K$ the conduction and the valence bulk subbands comprise pairs of $\varepsilon_i(p) \approx \beta_1 \pm vp \cos \left(\frac{i\pi}{N}\right)$ and pairs of $-\varepsilon_i(p) \approx -\beta_1 \pm vp \cos \left(\frac{i\pi}{N}\right)$, respectively, with
\(i = 1, 2, \ldots, \left\lfloor (N - 1)/2 \right\rfloor\), where \(\lfloor \cdot \rfloor\) is the Gaussian symbol. Besides, for even \(N\) they also comprise quadratic \(\varepsilon_{i=N/2}(p) \approx \beta_1 + (vp)^2/2\beta_1\) and \(\varepsilon_{i=N/2}(p) \approx -\beta_1 - (vp)^2/2\beta_1\), respectively. In each of the \(\left\lfloor (N - 1)/2 \right\rfloor\) pairs there is one conduction (valence) bulk subband extending downward (upward) from \(K\) towards the zero energy. It is just the subband \(\varepsilon_{j=N\rightarrow i}(p)\) \([-\varepsilon_{j=N\rightarrow i}(p)]\). Remarkably, it turns away around \(p_{D}\) and forms a valley as shown in Fig. 2. Such valleys are annular since all the eigenenergies are isotropic. According to Eq. (23), the turning is due to the nonlinear terms in powers of \(vp/\beta_1\) in the expansion of \(\pm \varepsilon_j(p)\).

There is an energy gap between the valley edges of the lowest downward conduction and the highest upward valence bulk subbands \(\pm \varepsilon_{j=N\rightarrow i}(p)\), which are the extensions from the aforementioned \(\varepsilon_{i=1}(p) \approx \beta_1 - vp \cos \left(\pi/N\right)\) and \(-\varepsilon_{i=1}(p) \approx -\beta_1 + vp \cos \left(\pi/N\right),\) respectively. By differentiating them in Eq. (23) with respect to \(vp\) near \(vp_{D}\), the edge momentum in ABC-stacked \(N\)-layer graphene is approximately given by

\[
p_{\text{edge}}^{(N)} = \beta_1/v \cos \left(\frac{\pi}{2N - 1}\right). \tag{31}\]

The edge energies of \(\pm \varepsilon_{j=N\rightarrow i}(p)\) are then obtained and so is the energy gap, the latter being

\[
\Delta_{\text{gap}}^{(N)} = 4\beta_1 \sin \left(\frac{\pi}{2N - 1}\right). \tag{32}\]

Equation (31) indicates that \(p_{\text{edge}}^{(N)}\) increases with increasing \(N\). In the course of the evolution, \(\Delta_{\text{gap}}^{(N)}\) diminishes as described by Eq. (32). The results displayed in Fig. 2 show that \(p_{\text{edge}}^{(N)}\) approaches \(p_{D}\) rapidly but as predicted, \(\Delta_{\text{gap}}^{(N)}\) approaches zero relatively slowly. A comparison in this aspect can be made with the case for AB-stacked graphene, whose band structure exhibits similar 3D features to AB-stacked graphite with just several layers \((N \approx 10)\). Taking the advantage of the explicit expression of \(\pm \varepsilon_j(p)\) given in Eq. (23), our calculation can be achieved for arbitrary \(N\). In Fig. 2, the energy gap at \(N \approx 100\) has become narrow, though still opening. For further realization of the evolution, the energy dispersion should also be investigated. The bulk subbands \(\pm \varepsilon_j(p)\) tend to disperse linearly in the increase of \(N\) as observed from Fig. 2. This tendency can be understood by analyzing the functionality of \(\cos \theta_j\) in Eq. (23).

The bulk DOSs \(D_{\text{bulk}}^{(N)}(\varepsilon)\) ranging from a few to dozens of layers and up to \(N \approx 100\) are also calculated and are shown in Fig. 3. There are as many peaks displayed in \(D_{\text{bulk}}^{(N)}(\varepsilon)\) as there are the bulk subbands. Each bulk subband yields a peak at its own valley edge. The most prominent two peaks are due to \(\pm \varepsilon_{j=N\rightarrow i}(p)\), separated by the aforementioned diminishing
gap $\Delta_{\text{gap}}^{(N)}$. Besides, a dip is present at energy $\beta_1 (-\beta_1)$ in the conduction (valence) bulk subband spectrum. This reflects the cusp at the $K$ point, where all the subbands are degenerate. All these features are gradually smeared in the evolution.

### B. Dimensional crossover

The dimensional crossover from the gapped bulk subbands in ABC-stacked graphene to the 3D Dirac cone structure in RG is elucidated with respect to Eq. (23). As $N \to \infty$, there exists an infinitely large subset of the $\lfloor (N - 1)/2 \rfloor$ downward (upward) conduction (valence) bulk subbands whose elements all approach

$$\pm \varepsilon_{\infty}(p) = \pm \beta_1 \mp vp,$$

where the values of respective $\theta_{N-1}$ all approach $\pi$ according to Eqs (24) or (25). The two limits given in Eq. (33) are two branches of the envelope described in Eq. (18), a necessary condition for the existence of the eigenvalues of $H^{(N)}_{\text{bulk}}(\varepsilon)$. They constitute the boundary of a zone containing the whole bulk subband spectrum for infinite $N$, which forms the continuum of the 2D projections from the 3D Dirac cone structure. They intersect at the infinite limit of the edge momentum $p^{(\infty)}_{\text{edge}}(= \beta_1/v)$ determined by Eq. (31), at which the energy gap closes up with $\Delta_{\text{gap}}^{(\infty)} = 0$ [see Eq. (32)]. Consequently, the bulk zone boundary forms a linear annular cone apexed along a circle at a distance $p_D(= \beta_1/v)$ from the $K$ point. The circle is known to be the 2D projection of the DP spiral as described in Eq. (2).

Using Eq. (23), the bulk subbands can be calculated for a huge number ($N$) of ABC-stacked graphene layers as desired. The results for $N = 1000$ are plotted in Fig. 4(a), in which the completely flat surface subbands are not plotted for brevity. As shown, the infinite limit has been practically attained. A gapless bulk zone full of bulk subbands are displayed. The zone boundary is, indeed, a linear annular cone with the apex located along a circle of radius $p_D$. The characteristics of the projected Dirac cones are also exhibited in the infinite limit of the bulk DOS $D^{(\infty)}_{\text{bulk}}(\varepsilon)$. The calculation results from Eq. (29) for $N = 1000$ are plotted in Fig. 4(b), shown to be consistent with the subband energies plotted in Fig. 4(a). Those features that are present for finite $N$, as shown in Fig. 3, are completely smeared in the infinite limit. In agreement with previous research, the results of $D^{(\infty)}_{\text{bulk}}(\varepsilon)$ acquired here is the same as the DOS in monolayer graphene, reflecting the characteristics of the
Dirac cone. In particular, the vanishing bulk DOS at the zero energy, viz., $D_{\text{bulk}}^{(\infty)}(0) = 0$, characterizes RG as a semimetal with half-filled DP spirals in the bulk.

V. SUMMARY AND OUTLOOK

The band structure of ABC-stacked $N$-layer graphene comprises flat surface and gapped bulk subbands as a consequence of the unique stacking configuration, where the non-trivial topology leads to a bulk-surface correspondence. So far, the intricate bulk subbands have not yet been unravelled, although the surface subbands are well understood. In this paper, for the first time ever the bulk subbands can be explicitly obtained for arbitrary $N$. Hence, their evolution with increasing $N$ can be demonstrated together with the surface subbands. The bulk subbands are certain 2D projections from the 3D Dirac cone structure at allowed wave vectors in the bulk of RG. Towards the infinite limit of the evolution, a bulk zone of the continuum of the 2D projections shows up and a dimensional crossover occurs from the gapped bulk subbands to the gapless 3D Dirac cone structure. Correspondingly, the surface subbands become completely flat within a region confined by the 2D projection of the DP spiral.

The physics with respect to ABC-stacking configuration for layered systems is rich and deep. As compared with the famous ABC-stacked layered 3D topological insulators such as Bi$_2$Se$_3$ and Bi$_2$Te$_3$, the 3D system RG here we focus on behaves as a topological semimetal. It possesses metallic flat surface subbands while being semimetallic in the bulk with a 3D Dirac cone structure. A generalization of the present study to other ABC-stacked systems is expected, regarding the evolution and dimensional crossover of the bulk subbands from 2D to 3D realm.

We point out the convenience of using an effective Hamiltonian closed in the bulk subspace. The resolution of the recursion involved in the eigenvalue problem can be achieved utilizing the nested structure of the effective Hamiltonian. An explicit expression of the bulk subbands for arbitrary $N$ can be thus obtained. Moreover, it is appropriate to construct an effective Hamiltonian that is non-perturbation in case the coupling between the surface and the bulk subbands is strong compared with a vanishingly small bulk energy gap for infinitely large $N$. 

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ACKNOWLEDGMENTS

This work was supported by the Ministry of Science and Technology of Taiwan, under the Grant nos. MOST 103-2811-M-165-001 and NSC 102-2112-M-165-001-MY3.

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**Figure Captions**

FIG. 1. (Color online) (a) Stacking configuration of ABC-stacked $N$-layer graphene. $B_1$ (black filled circles) and $A_N$ (black unfilled circles): surface sublattices; the rest (red circles): bulk sublattices. Nearest-neighbor TB hoppings ($\beta_i$) are shown; only $\beta_0$ and $\beta_1$ are used in the minimal model. (b) Solid view of the bulk lattice in RG, composed of infinitely many ABC-stacked graphene layers, with the biparticle rhombohedral primitive unit cell (red). An alternatively set hexagonal unit cell of triple volume (blue) is also plotted for reference. (c) Illustration of several 2D projections (red dots) of the DP spiral around $K$. The inset displays clockwise and counterclockwise DP spiraling senses with increasing $k_z$ around $K$ and $K'$, respectively.

FIG. 2. (Color online) Band structure of ABC-stacked $N$-layer graphene. Flat pair about the zero energy (grey): surface subbands; the rest (red): bulk subbands. The direction of the momentum is taken arbitrarily.

FIG. 3. (Color online) Bulk DOSs in ABC-stacked $N$-layer graphene, in the unit of number of states per $\beta_1$ per atom.

FIG. 4. (Color online) (a) Energies of the bulk subbands in ABC-stacked 1000-layer graphene, practically showing the dimensional crossover with the bulk zone full of bulk subbands. (b) Bulk DOS associated with (a), in the unit of number of states per $\beta_1$ per atom.
