Magnetoelectronic properties of the AB-stacked graphite

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Abstract

The tight-binding model is employed to study magnetoelectronic structures of the AB-stacked graphite. A specifically full band calculation on overall energy region is presented to compare with SWMcC method, which only concerns the magnetoelectronic structures along the HKH-axis. It is found that magnetoband structures, strongly depending on the perpendicular magnetic field ($B$) and the interlayer interactions, exhibit 0D, 1D and 2D characteristics at the strong magnetic field. The physical origin of 0D, 1D and 2D Landau levels is intensely discussed to show its speciality for graphite. Pronounced structures, including sharp peaks, square-root peaks, and logarithmic divergences, can be clearly found in the density of states (DOS). And the energy dispersions and DOS are specially sensitive to the magnitude of $B$: the lower the magnetic field is, the more Landau levels exist nearby Fermi energy ($E_F$). Meanwhile, the interlayer interactions significantly affect the state energies and the DOS features, e.g., peak position and peak shape. DOS in the form of sharp peak (square-root peaks) below (above) $E_F$ is expected to play an important role in such physical properties as absorption spectra.

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1. Introduction

Graphite is a layered crystal made up of hexagonal graphite sheets. The hexagonal networks of carbon atoms with sp$^2$ orbitals constitute a graphite sheet. And the remaining p$_z$ orbitals perpendicular to the plane, denoted as π states, dominate the physical properties at low energy. Two linear energy dispersions touch each other at Fermi energy. A graphite sheet is zero-gap semiconductor with vanishing density of states at Fermi energy. Graphite crystals are the arrangement of graphite sheets, e.g., AA, AB, or ABC sequence, along the z-axis. In general, natural graphite adopts an AB-stacking sequence [1–3]. The interlayer interactions are due to the van der Waals forces among the neighboring layers. They cause anisotropic energy dispersions along $k_z$ and play a crucial role in the energy dispersions at low energy [1–6]. Above all, the energy dispersions around the HKH-axis of the first Brillouin zone (FBZ) have been well described by the Slonczewski–Weiss (SW) band model [7].

SW band model is in some way useful in studying the band structures of the AB-stacked graphite in the vicinity of six vertical edges of FBZ. A 4 × 4 Hamiltonian matrix, based on the group theory, is so employed to study the energy dispersions. Around these axes, Hamiltonian matrix, by using ‘$k \cdot p$’ method, is expanded in power of the distance from the edge. And, the energy
dispersions are obtained [8]. The SW model is further extended by McClure (SWMcC model) to study the magnetoband structures along the HKH-axis of graphite under the magnetic field parallel to the $z$-axis [8]. Electronic states change into Landau levels in the graphite planes. Such Landau levels are coupled by the interlayer interactions along the HKH-axis. Many authors have ever made use of SWMcC model to study the Landau levels structures in graphite [9–15]. This method predicts the existence of Landau levels and a finite peak of density of states at Fermi energy $E_F$.

To deal with band structures of graphite, SW and SWMcC model are no doubt a convenient and practicable method because it is very easy to diagonalize a $4 \times 4$ matrix. SW model, however, can only offer the information of band structures of graphite at low energy. The electronic properties at high energy are lacking due to the limitation of SW model. Moreover, SW model only studies the energy dispersions along the HKH-axis, around which the electronic properties are isotropic. This result, in fact, is insufficiently to describe the properties of electrons moving along other directions in the momentum space. SWMcC method, the extension of SW model, only investigates magnetoband structures along the HKH-axis. Therefore, a full band calculation, which can fully and specifically describe Bloch electrons subjected to magnetic field, is expected.

To our knowledge, however, no study concerning the magnetoelectronic properties, including energy dispersions in the entire FBZ, has ever been presented. In this work, magnetoelectronic properties of the AB-stacked graphite are carefully studied within the Peierls-coupling tight binding model. Now firstly, the effects of magnetic field $B$ and crystal potential are both taken into account. And, full band calculation is performed; the related DOS is studied. This paper is organized as follows. In Section 2, the analytic Hamiltonian matrix elements of the tight-binding method for magnetoelectronic properties of AB-stacked graphite are first and most derived. The effects of magnitude of magnetic field and the interlayer interactions on the band dispersions are then investigated in Section 3. Following this, DOS of graphite is studied. Finally, conclusions are drawn in Section 4.

### 2. The tight-binding method

The geometrical structure of AB-stacked graphite is shown in Fig. 1. Half of carbon atoms, located at $A$ site, form a straight line along the $z$-axis, while others, at $B$ site, form a zigzag line in the $y-z$ plane. The distance between two nearest neighboring sheets is $c = 3.52 \text{ Å}$ [1]. The C–C bond length in graphite plane is $b = 1.42 \text{ Å}$. The atom–atom interactions shown in Fig. 1 are as follows. $\gamma_0$ represents the interaction between atom $A$ and $B$ atoms on the same graphite plane. The interlayer interaction between two $A(B)$ atoms from two neighboring layers is $\gamma_1(\gamma_3)$. The interaction from two next-neighboring plane is $\gamma_4(\gamma_2)$. $\gamma_4$ represents the interaction between atom $A$ and atom $B$, from two neighboring layers. $\gamma_6$ is the difference of the chemical environment between atom $A$ and atom $B$. The values of $\gamma_0$ and $\gamma_i$ are [1]: $\gamma_0 \approx 2.598 \text{ eV}$, $\gamma_1 \approx 0.364 \text{ eV}$, $\gamma_2 \approx -0.014 \text{ eV}$, $\gamma_3 \approx 0.319 \text{ eV}$, $\gamma_4 \approx 0.177 \text{ eV}$, $\gamma_5 \approx 0.036 \text{ eV}$, and $\gamma_6 \approx -0.026 \text{ eV}$.

In the presence of magnetic field perpendicular to graphite plane $B = (0,0,B)$, the Hamiltonian is $H = (\mathbf{P} - \frac{e}{c} \mathbf{A})^2 / 2m + V(\mathbf{r})$. The Bloch function of $\pi$ electron is expressed as

$$\Psi_{k,\alpha}(\mathbf{r}) = \frac{1}{\sqrt{N}} \sum_j \psi_{\alpha j}(\mathbf{r}) \times \exp \left( -i \frac{\mathbf{k} \cdot \mathbf{r} + \frac{e}{c\hbar} \int \mathbf{A}(\mathbf{R}, \mathbf{r}) \cdot d\mathbf{r}}{2m} \right)$$

where $\psi_{\alpha j}(\mathbf{R} - \mathbf{r})$ is the atomic-like wavefunction and $\alpha$ is atom site $A$ or $B$. $\mathbf{R}$ is the 3D periodical lattice vector. The vector potential is chosen as $\mathbf{A} = (0,0,B \mathbf{r})$ with the Landau gauge. The magnetic flux $\phi = 1/q$ ($q$ is a nonzero integer) through a hexagonal ring, in the unit of flux.
quantum $\phi_0 = \text{chle}$, puts a new periodicity with period $q$ on the Bloch electronics: $\Psi_1(r)_{x,m} = \Psi_1(r)_{x,m+q}$ $m(=1, \ldots ,q)$ labels the $m$th zigzag line along the $x$-axis in each graphite plane [Fig. 1]. Hence, there are 4$q$ electrons in the new primitive cell. Based on tight-binding model and the above-mentioned boundary condition, the $4q \times 4q$ Hamiltonian matrix is given by

$$
\begin{pmatrix}
B_{1,1} & B_{1,2}^* & 0 & \cdots & 0 \\
B_{2,1} & B_{2,2} & B_{2,3}^* & 0 & \cdots & 0 \\
0 & B_{3,1} & B_{3,2} & B_{3,3}^* & 0 & \cdots \\
0 & 0 & B_{4,1} & B_{4,2} & B_{4,3}^* & \cdots \\
\vdots & \vdots & \vdots & \ddots & \ddots & \vdots \\
0 & \cdots & \cdots & \cdots & 0 & B_{q,1} \\
B_{q,1}^* & 0 & \cdots & \cdots & 0 & B_{q,q}
\end{pmatrix}
$$

where $B_{ij}$ is a $4 \times 4$ block. The boundary conditions $B_{1,0} = B_{q,0}$ and $B_{q,q+1} = B_{1,1}^*$ are used to obtain Eq. (2). $B_{m,m}$ is spanned by four Bloch functions $1A_m$, $1B_m$, $2A_m$, and $2B_m$, where $1A_m$ and $1B_m$ $(2A_m$ and $2B_m)$ are at the $m$th zigzag line at the first (second) graphite plane. The matrix elements of Hermitian $B_{m,m}$ are expressed as follows:

$$
\begin{align*}
B_{m,m}(1, 1) &= \gamma_0 + \beta^2 \gamma_5/2, \\
B_{m,m}(1, 2) &= 2\gamma_0 \cos(k_x - \pi(m - [q])\phi) e^{-i k_y/2}, \\
B_{m,m}(1, 3) &= \gamma_1 \beta, \\
B_{m,m}(1, 4) &= 2\gamma_4 \beta \cos(k_x - \pi(m - [q] - \frac{1}{2})\phi) e^{i k_y/2}, \\
B_{m,m}(2, 2) &= \beta^2 \gamma_5/2, \\
B_{m,m}(2, 3) &= 2\gamma_4 \beta \cos(k_x - \pi(m - [q])\phi) e^{-i k_y/2}, \\
B_{m,m}(2, 4) &= \gamma_1 \beta e^{i k_y}, \\
B_{m,m}(3, 3) &= \gamma_0 + \beta^2 \gamma_5/2, \\
B_{m,m}(3, 4) &= 2\gamma_0 \cos(k_x - \pi(m - [q] + \frac{1}{2})\phi) e^{i k_y/2}, \\
B_{m,m}(4, 4) &= \beta^2 \gamma_5/2,
\end{align*}
$$

where $k_x$, $k_y$, and $k_z$ denote $\sqrt{3}b k_x/2$, $k_yb$, and $k_zc$, respectively. The wavevector is $k = (k_x, k_y, k_z)$. The matrix elements including $\beta(=2\cos(k_z))$ describe the interlayer interactions. $[q] = (q + 1)/2$ is included to set the origin of coordinate in the center of each period $q$ in the first graphite plane. It should be noted that $\phi//\psi$ is the Peierl’s phase shift caused by the magnetic flux passing half hexagonal ring. The $n\phi/3$ term in Eq. (2) is due to the difference between the centers of two neighboring graphite planes. The intralayer interaction $2\gamma_0 \cos(k_x - \pi (m - [q])\phi) e^{-i k_y/2}$, describing the interaction between $A$ atom and two nearest neighboring $B$ atoms at the same $n$th zigzag line, depends on position $m$ along the $y$-axis [Fig. 1]. The magnetic flux $\phi$ also changes wavevector from $k_x$ to $\{k_x - \pi(m - [q])\phi\}$. Apparently, the magnetic field modifies the periodic boundary condition of Bloch electrons in the $r$- and $k$-space.

The nonzero matrix elements of off-diagonal block $B_{m,m+1}$, with the relation $B_{m,m+1} = B_{m,1-m}^*$, are

$$
\begin{align*}
B_{m,m+1}(1, 4) &= \gamma_4 \beta e^{-i k_y}, \\
B_{m,m+1}(2, 1) &= \gamma_0 e^{-i k_y}, \\
B_{m,m+1}(2, 3) &= \gamma_4 \beta e^{-i k_y}, \\
B_{m,m+1}(2, 4) &= 2\gamma_3 \beta \cos(k_x - \pi(m - [q])\phi) e^{-i k_y/2}, \\
B_{m,m+1}(3, 3) &= \gamma_0 + \beta^2 \gamma_5/2, \\
B_{m,m+1}(3, 4) &= \gamma_0 e^{-i k_y}.
\end{align*}
$$

3. The magnetoelectronic properties

The energy dispersions of the AB-stacked graphite in the absence of magnetic field ($\phi = 0$) are shown in Fig. 1(b). Along HLAH [k = (k_x, k_y, \pi/2)] and $\beta = 0$, the interlayer interactions are closed. There are two independent graphite sheets. If the small $\gamma_0$ is neglected, then the state energies are the same as those of a single graphite sheet. The occupied states $E^-$ are symmetric to the unoccupied states $E^+$ about $E_F = 0$. There are linear bands and parabolic bands. At H, the interactions between $A(B)$ atom and its three nearest neighboring $B(A)$ atoms are closed. All the atoms in the graphite planes are in the isolated states. Here, all the electrons (or holes) can be regarded as free particles.

Along KH, interlayer interactions couple the isolated atoms. There are two types of atom chains in the system. One is a linear chain composed of $A$ atoms along the $z$-axis; the other is a zigzag chain made up of $B$ atoms in the $yz$-plane. These two chains are coupled by interaction $\gamma_4$. As a result, the energy dispersions along KH exhibit cosine bands and flat bands at $E_F$. The former originates in the linear atom chains. The latter is related to the zigzag atom chains. It is obviously found that the interlayer interactions cause quite different energy dispersions along $k_z$, i.e., the electronic structures act strongly anisotropic.
The interlayer interactions do play an important role in electronic properties. Along KMFK (k_z = 0, β = 2), the interlayer interactions are maximum. The occupied states \( E^c \) are asymmetric to the unoccupied states \( E^v \). The interlayer interactions destroy the state degeneracy and, thus, enhance the bandwidth. Bandwidth at Γ(A), for example, is 7(6)\( \gamma_0 \). The interlayer interactions also change the linear bands to parabolic bands around K point. In short, the interlayer interactions cause the anisotropic energy dispersions along \( k_z \). They also strongly modify the energy dispersions along \( k_x \), such as the enhance of bandwidth, the destroy of states degeneracy, and the change of linear bands to parabolic bands.

The magnetic field drastically modifies the electronic properties. The energy dispersions at \( \phi = 1/4 (=1/q) \) are shown by the heavy curves in Fig. 2(a). The relationship occurs between magnetic field \( B \) and flux via \( B = 79 \times 10^3 lq/T \). \( B \) is equal to \( 2 \times 10^4 (T) \) at \( \phi = 1/4 \). Such a field is too strong to experimentally produce. But, diagonalizing a 16 × 16 matrix is easy to work out. More importantly, the results provide us with a prompt way to understanding the characteristics of magnetoelectronic properties. Magnetic field groups the electronic states together and produces the Landau levels and oscillating Landau subbands. There are \( q = 4 \) groups of energy dispersions. They are asymmetric about \( E_F \). Along \( k,(k_z) \) energy dispersions mainly exhibit the Landau levels and oscillating Landau subbands, while there exist flat bands and parabolic bands along \( k_z \) (along XM). Energy dispersions act strongly anisotropic.

The properties of energy dispersions along \( k_x, k_y, and \ k_z \) are, respectively, discussed. Along \( \Gamma X'M \) [from \( k = (0, 0, 0) \) to \( k = (\pi/2, 0, 0) \)], 16 light curves are energy dispersions of \( E^c(k_x, 0, 0; \phi = 0), E^c(k_x + \pi/4, 0, 0; \phi = 0), E^c(k_x + \pi/2, 0, 0; \phi = 0) \), and \( E^c(k_x + 3\pi/4, 0, 0; \phi = 0) \), respectively. They are obtained through the zone-folding (ZF) method. The magnetic field \( \phi = 1/4 \) couples these 16 light curves and produces the Landau levels \( E^c(k_x, 0, 0; \phi = 1/4) \), as shown by heavy curves. It is clear that such energy dispersions \( E^c(k_x, 0, 0; \phi = 1/4) \) cannot be obtained by ZF method. There are eight occupied states \( E^c \) (unoccupied states \( E^v \)) due to two graphite sheets in the unit cell. The occupied states are asymmetric to the unoccupied states \( E^v \) about \( E_F \); i.e., the effect of interlayer interactions is energy-dependent.

Magnetic field drastically changes energy dispersions along \( Y' \) [from \( k = (0, \pi, 0) \) to \( k = (0, 0, 0) \)]. The light curves in Fig. 2(a) are energy dispersions \( E^v(0, k_y, 0; \phi = 0), E^v(\pi/4, k_y, 0; \phi = 0), E^v(\pi/2, k_y, 0; \phi = 0) \), and \( E^v(3\pi/4, k_y, 0; \phi = 0) \), respectively. There are flat bands and parabolic bands. They are asymmetric about \( k_y = \pi/2 \) because two graphite planes are not aligned along the \( y \)-axis. Energy dispersions \( E^v(0, k_y, 0; \phi = 1/4) \), shown by heavy curves in Fig. 2(a), are strongly modified by magnetic field. They are asymmetric about \( k_y = \pi/2 \), i.e., \( k_y \) is a good quantum number, which is the evidence that the magnetic field produces the periodic boundary condition along the \( y \)-axis. There are Landau levels and oscillating Landau subbands. For example, Landau level exists at \(-2.5\gamma_0 \) and \(-2.7\gamma_0 \). The strong oscillating Landau levels, meaning the delocalization of wavefunctions, exist near \( E_F \).

The interlayer interactions affect energy dispersions differently along X'M (along \( k_x \)), where \( \beta \) is changing from 2 to 0. The light curves are energy dispersions, \( E^c(0, 0, k_z; \phi = 0), E^c(\pi/4, 0, k_z; \phi = 0), E^c(\pi/2, 0, k_z; \phi = 0) \), and \( E^c(3\pi/4, 0, 0; \phi = 0) \), respectively. At \( M \), state energies are double degeneracy. They are corresponding to two independent graphite sheets. Along X'M, the interlayer interactions destroy the state degeneracy and lead to cosine bands and partial flat bands. Magnetic field \( B (\phi = 1/4) \) destroys the state degeneracy at \( M \) due to the phase difference \( \pi \phi/3 \) [Eq. (2)] between two graphite planes. \( B \) alters the energy dispersions along X'M. There exist partial flat bands, Landau levels and cosine bands.

![Fig. 2. (a) The light curves exhibit the energy dispersions \( E^c(k_x, k_y, 0; 0) \), \( E^c(k_x + \pi/4, k_y, 0; 0) \), \( E^c(k_x + \pi/2, k_y, 0; 0) \), and \( E^c(k_x + 3\pi/4, k_y, 0; 0) \), respectively. The heavy curves exhibit the energy dispersions \( E^c(k_x, k_y, 1/4) \). (b) The energy dispersions at \( \phi = 1/40 \). The length of \( \Gamma X' \) is scaled the same as \( \Gamma X' \) in (a) for the sake of comparison.](image)
The characteristics of energy dispersions are dwelt on as follows. First, the interlayer interactions are closed. Two graphite sheets are decoupled in the unit cell. At \( k = (\pi/8, 0, \pi/2) \), \( B_{m,n}(1,2) \) in Eq. (2) is equal to zero at \( m = 1, 5, 9, \ldots \) chains. The magnetic flux cuts the first graphite sheet along such zigzag chains. Consequently, there are many identical strips with period \( q = 4 \) in the real space. Each identical strip contains three zigzag lines with two dangling bonds attached to the cusps positions of the outmost zigzag lines. State energies are \( \pm 2.59/\gamma_0, \pm 1.83/\gamma_0, \pm 1.38/\gamma_0, \) and \( \pm 0.15/\gamma_0 \) respectively. The wavefunction related to \( E = \pm 2.59/\gamma_0 \) has zero amplitude at the dangling bonds and large amplitude at the inner three zigzag lines, while the wavefunction of \( E = \pm 0.15/\gamma_0 \) is mainly located at the dangling bonds. From \( \Gamma \) to \( X' \), the intralayer interaction \( [B_{m,n}(1,2)] \), which is dependent on \( k_x \), begins to couple the neighboring strips. This brings about the \( 2 \times 4 \) oscillating Landau subbands. The nonvanishing intralayer interaction \( B_{m,n}(1,2) \) \( [2/2 \cos(k_x - \pi(m - [q])\phi)] \) connects the dangling bonds in the neighboring identical strips. The strong interactions between neighboring dangling bonds induce the widest Landau subbands near \( E_F \). The drastic oscillations of Landau subbands reflect the delocalization of wavefunctions. However, the less overlap of the wavefunctions of the neighboring strips, the narrower Landau subbands. Apparently, the second graphite sheet has the same energy dispersions with a phase shift \( \pi/12 \), which results from \( \pi\phi/3 \) in Eq. (3) \( [B_{m,n}(1,4) \) in Eq. (3)]. Landau subbands exhibit 0D and 2D characteristics in a graphite plane. Such magnetoband features originate in the specially geometric structure on the graphite plane. Then, the interlayer interactions couple these two graphite sheets. They generate \( 2 \times 2 \times 4 \) oscillating Landau subbands along \( k_x(k_y) \) and induce energy dispersions along \( k_z \), which exhibit partial flat bands, flat bands and cosine bands. It is found that energy dispersions along \( k_z \) have a strong atomic-site dependence. Cosine bands (flat bands) are related to linear atom chains made up of \( A \) atoms along the \( z \)-axis (zigzag atom chain composed of \( B \) atoms in the \( yz \)-plane). Partial flat bands are the hybridization of cosine band and flat band. Above all, these band features, including 0D, 1D and 2D Landau levels discussed above, will be reflected on DOS.

Now, it is also found that the magnitude of magnetic field greatly influences energy dispersions. Fig. 2(b) exhibits the energy bands at \( \phi = 1/40 \) \( [B = 2 \times 10^5 \text{ T}] \), which are similar in shape to those at a very low magnetic field. Nevertheless, we may have no other choice but to diagonalize a 20,000 \( \times \) 20,000 matrix, for example, at \( B = 15.8 \) (T). To diagonalize such a large matrix is only possible at the cost of a large amount of CPU running time. As a matter of convenience, magnetoelectronic properties at large \( \phi \) are illustrated in this work. At \( X' \), \( k \) is equal to \( (\pi/40, 0, 0) \). For the sake of comparison, its length is scaled the same as \( X' \) in Fig. 2(a). There are Landau levels along \( k_x \) and \( k_y \), while there exist cosine bands and partial flat bands along \( k_z \). At \( M \) \( (k = (\pi/40, 0, \pi/2) \) and \( \beta = 0 \), there exists the zero energy point. The interaction \( B_{m,n}(1,2) \approx 0 \) [Eq. (2)] at \( m = 1 \) zigzag line; that is to say, the magnetic flux cuts the first graphite plane at the \( m = 1, 41, 81, \ldots \) zigzag line and produces the zero energy point. The state energies at \( E_F \) with weak dispersion along \( X'M \) are due to interlayer interactions \( \gamma_2 \) and \( \gamma_5 \). It should be noticed that there are almost dispersionless state energies at energy region \( E \leq \gamma_0 \), which exhibit the 0D characteristic. Such a localized state (Landau level) will give rise to a sharp peak in DOS.

The Butterfly-like spectra are shown in Fig. 3(a). They are state energies at \( \Gamma, \gamma, \phi \), where \( q \) is the inverse of magnetic flux \( \phi \). Due to the effect of lattice potential, the state energies exist at energy region between \( -\gamma_0 \) and \( 4\gamma_0 \). At high magnetic field \( (\phi_0/\phi < 50 \{ B > 1580 \text{ (T)} \}) \), the discrete energy states are clearly found. However, \( E(\gamma_0) \) \[ Eq. (2) \] between \( 2\gamma_0 \) and \( 4\gamma_0 \) \[ Eq. (2) \] gradually become continuous states with the decrease of magnetic flux \( (\phi_0/\phi > 100 \{ B < 790 \text{ (T)} \}) \). Fig. 3(b) shows the Butterfly-like spectra at a low energy region. The discrete state energies at \( E < 0.5|\gamma_0| \) can be clearly observed. The energy spacing between two neighboring Landau levels is not the same because the Bloch electrons undergo both the magnetic field and crystal potential. This fact also strongly implies that the model of free electrons in the magnetic field is inadequate to simulate this system.

In Fig. 3(c) and (d), the energy dispersion near \( E_F \) at \( \phi = 1/200 \) \[ \{ B = 395 \text{ (T)} \] and \( \phi = 1/500 \) \[ \{ B = 158 \text{ (T)} \] along the HKH-axis \[ \{ 2\pi/3, 0, -\pi/2 \} \] to \[ \{ 2\pi/3, 0, \pi/2 \} \] are shown, respectively, to illustrate the effect of interlayer interactions. There are parabolic bands and nearly dispersionless bands at \( E_F \). The main feature of the energy dispersions remains so unchanged for the variation of magnetic flux. However, the state energies are actually sensitive to the magnitude of magnetic field. At \( H \), the interlayer interactions are closed except \( \gamma_0 \). Two levels at \( E_F \) are split due to \( \gamma_0 \). Moreover, there exist many extrema in levels at \( H \). They are Landau levels of a graphite sheet in the presence of magnetic field. A special feature of these levels is the unequal Landau level spacing. From \( H \) to \( K \), the interlayer interactions significantly destroy the state degeneracy and change the state energies. These effects are mainly caused by \( \gamma_1 \), the interactions between \( A \) and \( A \) atoms from the neighboring planes. The interactions \( \gamma_1 \) and \( \gamma_4 \) also cause the energy dispersions to seriously cross (or anticross) and, thus produce many extrema. The higher the state energy is, the more extrema appear. The positions of extrema are strongly dependent on the state energy of Landau levels. So, the extrema increase with the decrease of magnitude of magnetic field. Nakao reported that many extrema...
appear near $H$ at a very low magnetic field. The origin of extrema is discussed in connection with the magnetic breakthrough effect caused by $\gamma_A$, the interactions between atoms $A$ and $B$ from the neighboring planes, near the H-point [10]. More specially, the shape of levels at $E_F$ in Fig. 3(d) is clearly modified at the low field. The chief cause is that the levels at $E_F$ are strongly affected by the Landau levels in the vicinity of $E_F$ through the interlayer interaction at a low magnetic flux.

The properties of magnetoband structures also reflect on DOS. DOS is evaluated by $D(\omega) = \sum_{k,h} |\nabla_k E^@k(\mathbf{k},\phi)|^3 |\omega|$. DOS mainly exhibits four kinds of special structures: discontinuities, logarithmic divergences, power-law divergences and a delta-function-like divergence, which are, respectively, due to the minimum or maximum of energy bands, the saddle point in energy bands, the flat bands along two directions and the parabolic band along the third direction, the flat bands along three directions. The dashed curve in Fig. 4(a) shows DOS of the AB-stack graphite at $\phi = 0$. DOS is asymmetric about $\omega = 0$ due to the energy-dependent interlayer interactions. It is featureless at $|\omega| > 2\gamma_0$. There are two kinds of special structures in DOS: logarithmic divergences and discontinuities. For example, logarithmic divergence (discontinuity) is at $\omega = 0.9\gamma_0$ ($\omega = -3.2\gamma_0$). The former (latter) comes from the saddle points (the maximum or minimum of energy dispersions) in band [Fig. 1(b)].

Magnetic field modifies the electronic states and, thus, produces the discrete Landau peaks in DOS. DOS at $\phi = 1/4$ is shown by the heavy line in Fig. 4(a). It is asymmetric about $E_F$. There are $2 \times 4$ Landau peak. Each Landau peak owns two subpeaks due to the existence of two graphite planes in the unit cell. DOS chiefly exhibits the delta-function-like divergences, the power-law divergences, the logarithmic divergences and the oscillating structure. The delta-function-like divergences, which show an 0D characteristic, for instance, at $-2.7\gamma_0$, are related to the partial flat bands along $\hat{z}$ and the Landau levels along $\tilde{k}_z$ and $\tilde{k}_y$ [Fig. 2(a)]. The power-law divergence at $3.4\gamma_0$ is a 1D state, which results from the parabolic band along $\tilde{k}_z$ and the flat bands along $\tilde{k}_z$ and $\tilde{k}_y$. The oscillating structures at energy region $|\omega| \lesssim 0.5\gamma_0$, exhibiting a 2D property, come from the flat bands along $\tilde{k}_z$ and the oscillating Landau levels along $\tilde{k}_z$ and $\tilde{k}_y$.

DOS, as you see, is greatly affected, too. DOS at $\phi = 1/40$ is shown by the light curve in Fig. 4(a). Clearly, there are more Landau peaks in DOS as the magnitude of magnetic field decreases. So the peak heights and
positions are strongly dependent on the magnetic flux. There are three kinds of structures in DOS: power-law divergences, logarithmic divergences, and delta-function-like divergences. For instance, the delta-function-like divergence at \( x = 0 \) is related to Landau levels along \( ^\mathbf{k}_x, ^\mathbf{k}_y \) and \( ^\mathbf{k}_z \).

The property of DOS at low energy region vs. magnetic flux \( \phi \) deserves a closer investigation. Fig. 4(b) shows DOS at \( \phi = 0, \phi = 1/4, \phi = 1/20 \) and \( \phi = 1/40 \), respectively. At \( \phi = 0 \), nonzero amplitude of DOS at \( \omega = 0 \) exhibits the character of metal. It is attributed to the contribution of flat bands at \( E_F \) along \( ^\mathbf{K}H \) [Fig. 1(b)]. The very strong magnetic field \( (\phi = 1/4) \) produces a widely oscillating band at energy region \( |\omega| \leq 0.5\gamma_0 \). As the magnetic flux decreases to \( \phi = 1/20 \), a delta-function-like divergence appears at \( E_F \) [the light-dashed curve]. More delta-function-like divergences with the relatively weak amplitude occur near \( E_F \) at \( \phi = 1/40 \) [the light curve]. It is remarkable that there are sharp peaks (square-root peaks) below (above) \( E_F \) in DOS. The former (latter) belongs to 0D (1D) state. They are asymmetric about \( E_F \) due to the effect of interlayer interactions. It is deduced that the lower the magnetic field is, the more delta-function-like divergences (square-root peaks) exist at a low energy region. Moreover, the amplitude of these delta-function-like divergences (square-root peaks) will become smaller as the magnitude of magnetic field decreases. Such peaks near \( E_F \) are expected to have significantly effects on low-energy absorption spectra.

4. Conclusions

The exact Landau levels and related DOS of AB-stacked graphite are studied in the Peierls-coupling tight-binding method. The effects of magnetic field \( B \) and crystal potential are treated at the same footing. It is shown that the Landau levels of Bloch electrons are strongly affected by the crystal potential (intralayer and interlayer interactions). Especially, the Landau levels near the Fermi energy are very sensitive to the crystal potential. Moreover, energy dispersions along \( ^\mathbf{k}_z \) and \( ^\mathbf{k}_x \) are, respectively, completely studied. To put it differently, a full band calculation is performed. Thus, the magneto-electronic properties at full energy region can be studied in detail. The above-mentioned tasks cannot be accomplished by only adopting SWMcC model.

Peierls-coupling tight-binding method allows us to see the problem with ready insight. The magneto-electronic properties are strongly dependent on the interlayer interactions and the magnitude of \( B \). On one hand, \( B \) modifies the crystal potential (intralayer interaction) through the Peierls phase induced by \( B \), and then establishes a new boundary conditions on Bloch electrons in real and momentum space. In this way, Landau levels of Bloch electrons generate. \( B \) effectively changes the band structures, such as energy dispersions, energy spacing, bandwidth and the oscillation period of Landau level. On the other hand, the interlayer interactions, originating in the stacked system, couple these Landau levels along the \( ^\mathbf{z} \)-axis, and therefore, produce the \( ^\mathbf{k}_z \)-dependence energy dispersions. The interlayer interactions significantly modify energy dispersions, energy spacing, bandwidth and oscillation period of Landau levels.

As is remarkably shown, \( B \) reduces the dimensionality of AB-stacked graphite while the interlayer interactions have opposite effects. And above all, the competition of the crystal potential and magnetic field may diversify the magneto-electronic properties. The energy dispersions exhibit 0D, 1D and 2D characteristics at the very strong magnetic field. The related sharp peaks, square-root peaks, and logarithmic divergences are clearly found in DOS. The energy dispersions are greatly affected and, the lower the magnetic field is, the more Landau levels exist. The delta-function-like divergences (power-law divergences due to interlayer interactions) at the low energy region can be finally discovered and proved at low magnetic field.
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