Electronic spectrum of twisted bilayer graphene: from insulator to metal

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We study the electronic properties of twisted graphene bilayers in the tight-binding approximation, taking into account the nearest-neighbor hopping of electrons in each graphene plane. The interlayer hopping amplitude is modeled by a function, which depends not only on the distance between two carbon atoms, but also on the positions of neighboring atoms as well. Using the Lanczos algorithm for the numerical evaluation of eigenvalues of large sparse matrices, we calculate the bilayer single-electron spectrum for commensurate twist angles in the range $1^\circ \lesssim \theta \lesssim 20^\circ$. We show that the bilayer may experience a metal-insulator transition at $\theta_c \approx 1.89^\circ$. For large angles, the electronic spectrum has a gap. At small angles the system is a metal with a well-defined Fermi surface.

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Introduction— Bilayer graphene is attracting considerable attention. Recent experimental studies (including scanning tunneling microscopy [1,2], Raman [3,4], and angular resolved photoemission spectroscopy [5,6,7,8]) revealed that, in many cases, the structure of bilayer samples is far from the ideal AB stacking and is characterized by a non-zero twist angle $\theta$ between graphene layers. The physics of twisted bilayer graphene (tBLG) is very rich, including Dirac spectrum with a $\theta$-depended Fermi velocity [9,10], low-energy van Hove singularities [11,12], and other anomalies [13,14].

The specific electronic properties of the tBLG are mostly determined by the interlayer single-electron hopping and the twist angle. Commensurate structures with characteristic Moiré superlattices exist only for a discrete set of angles $\theta$. In this case, numerical studies were performed based on density functional theory and tight-binding calculations [11,13]. Since the elementary unit cell of the tBLG superlattice contains a large number of sites, especially at small twist angles, the $\textit{ab initio}$ calculations incur a significant computational cost.

To avoid this difficulty, several semi-analytical theories have been developed for describing the low-energy electronic properties of the tBLG [10,21]. These theories operate mainly with the electronic states near the Dirac cones, which the tBLG inherits from its two constituent layers. In the tBLG, the Dirac cones with equal chirality are located close to each other in momentum space. The interlayer hopping couples these cones and suppresses the Fermi velocity [11,12]. When the twist angle is small ($\theta \lesssim 2^\circ$), the picture with Dirac cones becomes irrelevant. Instead, the system acquires a finite density of states at the Fermi level [16]. However, the electronic spectrum was not properly analyzed in the regime of small $\theta$. The approach proposed in [21] includes a finite mass term in the effective long-wave Hamiltonian of the tBLG. The electronic spectrum obtained is gapped or gapless depending on the type of commensurate structure. However, the types of spectra predicted in [21] do not coincide with those obtained in other low-energy theories, e.g., [17,18]. Thus, despite definite progress, a commonly-accepted picture of the electronic structure of the tBLG is still absent.

Here we report the results of tight-binding calculations of the band structure of tBLG in a wide range of twist angles. To tackle the issue of the large supercell size, which becomes a significant difficulty for small $\theta$, we use the Lanczos algorithm. This allows us to calculate the low-energy spectrum of tBLG. We find that the tBLG is an insulator with a gap in the electronic spectrum, if $\theta \gtrsim \theta_c \approx 1.89^\circ$. The gap is estimated as 80 meV, for $\theta = 20^\circ$. The gap decreases with decreasing $\theta$. At a critical angle $\theta_c$, a metal-insulator transition occurs. The system has a well-defined Fermi surface in the metallic phase.

Geometrical considerations.— Each graphene layer in the tBLG consists of two sublattices ($A_1, B_1$ in the layer 1, and $A_2, B_2$ in the layer 2). The positions of the carbon atoms in each sublattice in the bottom layer 1 are $r_n^A = r_n = n a_1 + m a_2$, $r_n^{1B} = r_n + \delta_1$, where $n = \{n, m\}$ (n, m are integers), $\delta_1 = (a_{1,2})/3 = a\{1/\sqrt{3}, 0\}$, and $a_{1,2}$ are basis vectors of the graphene elementary unit cell, $a_1 = a\{\sqrt{3}, -1\}/2$, $a_2 = a\{\sqrt{3}, 1\}/2$, with the lattice parameter $a = 2.46\, \text{Å}$. The distance between graphene layers is $d = 3.35\, \text{Å}$. When the layers are not rotated ($\theta = 0$), the system is a perfect AB bilayer.

Layer 2 is rotated with respect to layer 1 by the angle $\theta$ around the axis connecting the atoms $A_1$ and $B_2$ with $n = 0$ (see Fig. 1). In this case the atoms of the top layer have the positions $r_n^{2B} = r_n = n a_1^t + m a_2^t$, $r_n^{2A} = r_n - \delta_2$, where $a_{1,2}^t = a_{1,2} (\cos \theta \pm \sin \theta / \sqrt{3}) \pm a_{2,1} (2 \sin \theta / \sqrt{3})$, and $\delta_2 = a\{\cos \theta, \sin \theta\} / \sqrt{3}$. 
infinite set of commensurate angles with different
layer by an angle
for a given

\[ \sin \theta, \cos \theta \]

The electronic spectra presented in Fig. 2 are calculated along the
Dirac point

\[ K \]

\[ K' \]

\[ K'' \]

Fig. 1(b). It has the shape of a hexagon with sides

\[ \Delta K = |K_\theta - K| \]

where \( K = 4\pi \{0, 1\}/3 \) and \( K_\theta = 4\pi \{-\sin \theta, \cos \theta\}/3 \) are the Dirac points of the bottom and top layers, respectively.

The structure of the tBLG is commensurate if

\[ \cos \theta = \frac{3m_0^2 + 3m\sigma r + r^2/2}{3m_0^2 + 3m\sigma r + r^2}, \]

where \( m_0 \) and \( r \) are mutually prime positive integers. The number of sites in the elementary unit cell of the so-called Moiré superlattice is equal to

\[ N = 4(3m_0^2 + 3m\sigma r + r^2) \]

if \( r \neq 3n \) (\( n \) is integer), or

\[ N = 4(3m_0^2 + m\sigma r + r^2/3) \]

otherwise. The size of the superlattice is \( L \sim a\sqrt{N} \) and, for a given \( m_0 \), the superstructure has a smallest size if

\[ r = 1. \]

It is seen from Eq. (1) that in the vicinity of the angle \( \theta \), corresponding to some \( m_0 \) and \( r = 1 \), there is an infinite set of commensurate angles with different \( m_0' > m_0 \) and \( r' > 1 \). These structures have larger superlattice-size cell. However, as it was shown in Ref. [18], such structures are almost periodic repetitions of the structure with \( m_0 \) and \( r = 1 \). For this reason we study here only the case \( r = 1 \).

If \( r = 1 \), the basis vectors of the superlattice are

\[ R_1 = m_0a_1 + (m_0+1)a_2, R_2 = -(m_0+1)a_1 + (2m_0+1)a_2. \]

The basis vectors of the reciprocal superlattice can be written as

\[ G_1 = 4[(2m_0+1)b_1 + (m_0+1)b_2]/N \]

and

\[ G_2 = 4[-(m_0+1)b_1 + m_0b_2]/N, \]

where \( b_1, b_2 = 2\pi \{1/\sqrt{3}, \pm 1\}/a \) are the reciprocal lattice vectors of the bottom layer. The first Brillouin zone of the superlattice is shown in Fig. 1(b).

Tight-binding Hamiltonian.— It is convenient to enumerate sites in the sublattice in each layer using two integer-valued vectors \( j = \{i, j\} \) and \( n = \{n, m\} \), where \( j \) marks the position of the supercell in the lattice, while \( n \) enumerates the sites inside the supercell. Then, we can write down the tight-binding Hamiltonian of the tBLG in the form

\[ H = -t \sum_{\langle i, j \rangle \in \Lambda} \left( \begin{array}{c} \sum_{\sigma} d_{i\sigma}^\dagger d_{j\sigma} + H.c. \end{array} \right) + \]

\[ \sum_{\langle i, j \rangle \in \Lambda} \left( \begin{array}{c} \sum_{\sigma} \left[ t_{\delta}^\alpha(R_i + r_{n}^\alpha; R_j + r_{m}^\beta) d_{i\sigma}^\dagger d_{j\sigma} + H.c. \right], \end{array} \right) \]

where \( R_j = iR_1 + jR_2 \), the symbol \( \langle \ldots \rangle \) stands for summation over the nearest neighbors, \( d_{i\sigma}^\dagger \) and \( d_{j\sigma} \) are the creation and annihilation operators of an electron with the spin projection \( \sigma \) in the layer \( s = (1, 2) \) on the sublattice \( \alpha = A, B \) in the supercell \( j \) in the position \( n \) (the position of this site is \( R_j + r_{n}^\alpha \)). The first term describes the in-plane nearest-neighbor hopping with amplitude \( t = 2.57 \) eV. The second term describes the interlayer hopping with \( t_{\perp} \) being the hopping amplitude between sites in the positions \( r \) and \( r' \).

This Hamiltonian is invariant with respect to translations on the vectors \( R_{1,2} \). Performing the Fourier transform \( d_{k\sigma} = N_{sc}^{-1/2} \sum_{ij} e^{-ikR_{ij}} d_{j\sigma} \), where \( N_{sc} \) is the number of supercells in the bilayer, and using the relation

\[ t_{\perp}(R_j + r; R_j + r') = t_{\perp}(r; r'), \]

we obtain

\[ H = \sum_{knm} \left( \begin{array}{c} \sum_{\sigma} \left[ t_{\delta}^\alpha(k) d_{k\sigma}^\dagger d_{k\sigma} + H.c. \right] + \right. \right. \]

\[ \left. \left. \sum_{\delta} \left[ t_{\delta}^\alpha(k) d_{k\sigma}^\dagger d_{k\sigma} + H.c. \right], \right) \right), \]

where \( k \) runs over the first Brillouin zone of the superlattice. In Eq. (3),

\[ t_{nm}^\alpha(k) = -t \sum_{j\delta} e^{-ikR_{ij}} \delta_{N_j + n, m - \delta}, \]

\[ t_{\perp}^\alpha(k) \]

\[ = \sum_{j} e^{-ikR_{ij}} t_{\perp}(R_j + r_{n}^\alpha; r_{m}^\beta), \]

\[ \delta \]

takes the values \( \{0, 0\}, \{1, 0\}, \{0, 1\}, \) and \( \{m_0i - (m_0 + 1)j, (m_0 + 1)i + (2m_0 + 1)j\} \). We use the approach proposed in [22] to calculate the interlayer hopping amplitudes. The main premise of this approach is that \( t_{\perp}(r; r') \) depends not only on the relative positions of the initial and final carbon atoms, but also on the positions of other atoms in the bilayer via the screening function \( S(r; r') \) (see Eq. (2) in [22]); the closer some of the neighboring atoms are to the line connecting the sites \( r \) and \( r' \), the larger is the screening. The inclusion of the screening is very important. Otherwise, the longer-range hopping amplitudes in the usual
Slonczewski-Weiss-McClure (SWM) scheme cannot be correctly reproduced.

Following Ref. [22] we present the hopping amplitude in the form $t_{\pm}(r; r') = [d^2 V_\sigma(r; r') + (r - r')^2 V_\pi(r; r')]/(d^2 + (r - r')^2)$, where $V_\sigma$ and $V_\pi$ are given by Eq. (1) in [22]. We found that the contribution to $t_{\pm}$ from $V_\pi$ is negligible, in agreement with Refs. [17, 18]. Due to screening, the function $t_{\pm}(r; r')$ decays very quickly when $|r - r'| > a$. The functions $V_\sigma(r; r')$ and $S(r; r')$ in [22] depend on seven fitting parameters ($\alpha_{1,2,3,4}$ and $\beta_{1,2,3}$). However, the values found in [22] cannot be directly applied to bilayer graphene [13].

Instead, we use the following estimates for the fitting constants [23]: $\alpha_1 = 6.715$, $\alpha_2 = 0.762$, $\alpha_3 = 0.179$, $\alpha_4 = 1.411$, $\beta_1 = 6.811$, $\beta_2 = 0.01$, and $\beta_3 = 19.176$ (c.f. with the third line of Table 1 of Ref. [22]). Performing the fitting procedure of [22] with these coefficients we reproduce the well-known SWM hopping amplitudes $\gamma_{1,3,4}$ in the AB bilayer (see Fig. 1 for the definitions of $\gamma_{1,3,4}$).

We introduce the $N$-component operator $\Psi_{\nu k} = \{d_{knA}, d_{knB}, d_{knA}^\dagger, d_{knB}^\dagger\}$ and rewrite Eq. (3) in the form $H = \sum_{\nu k} \Psi_{\nu k}^\dagger \tilde{H}_{\nu k} \Psi_{\nu k}$, where the $N \times N$ matrix $\tilde{H}_{\nu k}$ is constructed from $t_{\nu mn}(k)$ and $t_{\nu m\beta}^\dagger(k)$ according to Eq. (4). The energy spectrum of the tBLG consists of $N$ bands $E^{(i)}_{\nu k}$ ($i = 1, \ldots, N$). We are interested here in the spectrum near the Fermi level $\mu$ at half-filling. The chemical potential $\mu$ may be non-zero due to the violation of the particle-hole symmetry in Eq. (3). The value of $\mu$ is obtained from the usual equation $\sum_{\nu k} \int d^2 k \Theta(\mu - E^{(i)}_{\nu k})/\nu_{BZ} = 2$, where $\nu_{BZ}$ is the area of the first Brillouin zone of the supercell. Our calculations show [28] that $|\mu|$ is very small for any twist angle $\theta$, and only four bands with the smallest absolute values, $E^{(i)}_{\nu k} = E^{(i+\nu)}_{\nu k}$ ($i_0 = N/2 - 2, \nu = 1, \ldots, 4$) can cross the Fermi level.

The distant hopping amplitudes turn out to be negligible, and the matrix $\tilde{H}_{\nu k}$ is very sparse, that is, the number of non-zero elements in $\tilde{H}_{\nu k}$ is proportional to $N$. This allows us to use the Lanczos algorithm to calculate the eigenvalues closest to zero energy [29]. Then we calculate the spectra along the contour in the $k$ space shown in Fig. 1(b) for a set of $m_0$ varying from $m_0 = 1$ ($\theta = 21.787^\circ$, number of sites in the supercell $N = 28$) to $m_0 = 25$ ($\theta = 1.297^\circ$, $N = 7804$). The results for three different angles are shown in Fig. 2(a)–(c). When $m_0 < 17$, two pairs of bands come close to the Fermi level $\mu$ in the vicinity of the Dirac points $K$ and $K_\theta'$: one pair from below and another pair from above. The bands in each pair are almost degenerate in a large range of momentum space. The smaller $\theta$ is, the smaller is the energy difference between bands in these pairs.

Insulating phase. — If $\theta > \theta_c \approx 1.89^\circ$ ($m_0 < 17$), neither of the bands reach the Fermi energy. Thus, in this case, the system is an insulator with a non-zero band gap $\Delta$. Near the Dirac points $K$ or $K_\theta'$ the energy spectrum can be approximated as

$$E^{(i)}_{\nu k + \delta k} = \mu \pm \sqrt{\Delta^2 + v_F^2 (|\delta k| + k_{0i})^2},$$

where different signs correspond to different bands; $\Delta$, $v_F$, and $k_0$ are fitting parameters [see Fig. 2(d, e)]. The dependence of $\Delta$ and $v_F$ on the angle $\theta$ calculated by fitting $E^{(i)}_{\nu k}$ with Eq. (6) are shown in Fig. 3. The gap monotonously decreases when $\theta$ decreases, with a single exception at $\theta = 9.43^\circ$. The gap $\Delta \geq 1 \text{K}$, if $\theta \geq 4.408^\circ$ ($m_0 \leq 7$) and achieves the value $\Delta = 0.08 \text{eV}$ when $\theta = 21.787^\circ$ ($m_0 = 1$). Thus, it can be experimentally measured if the twist angle is not small. The spectrum of the tBLG with a gap was observed in recent experiments [8]. However, the nature of this gap is unclear.

If we neglect the values $\Delta$ and $k_0$ in Eq. (6), the band structure reduces to two doubly-degenerate Dirac cones located at the points $K$ and $K_\theta$ and intersecting at higher energies. The Fermi velocity $v_F$ is smaller than that in the single layer graphene, $v_{0F}$. This picture is quite consistent with many previous studies utilizing different approaches [11, 19].

The gap formation may be attributed to hybridization between the states located near the Dirac cones $K_\theta$ and $K'$ ($K$ and $K'_\theta$). Indeed, for commensurate structures, the momentum $K'$ is equivalent to $K_\theta$ because $K' = K_\theta + (2m_0 + 1)G_2$ [see Fig. 1(b)]. Thus, the corresponding hopping amplitude is non-zero, and the states near $K_\theta$ and $K'$ are mixed, which leads to the gap opening. This hybridization is ignored in the continuum approximations [17, 18], even though [17, 18] mentioned such a possibility. The phenomenological approach taking into account the hybridization between different Dirac cones in the tBLG was proposed in [20]. However, if $r = 1$, as we assume in this paper, the formalism of [20] predicts a gapless spectrum, failing to capture the insulating state of the tBLG. The tight-binding calculations in Ref. [12] predict the existence of the gap in the tBLG. However, the value of this gap is at least one order of magnitude smaller than our value (c.f. Fig. 4 with Fig. 9 in [12]). We attribute this discrepancy to the different choice of the function $t_{\pm}(r; r')$. We believe that our choice is more suitable for the tBLG since it reproduces SWM hopping parameters for AB bilayer graphene. A similar conclusion was reached in Ref. [21].

### Metallic phase

The Fermi velocity $v_F$ calculated according to Eq. (6) decreases when $\theta$ decreases (see Fig. 3), in good agreement with previous theoretical studies [11, 15, 17, 18], as well as with experimental observations [1, 2].

For angles close to $\theta_c = 1.89^\circ$, four low-energy bands become almost flat in the whole Brillouin zone with the exception of the small region near the point $M$ [see Fig. 2(a–c)]. For smaller angles, $\theta < \theta_c$ ($m_0 > 17$), the cone-like shape of the low-energy bands completely disappears even near the Dirac points [see the inset of Fig. 2(c)], the gap becomes zero, and the system acquires a Fermi
FIG. 2: (Color online) (a)–(c) The spectra of the tBLG calculated for three different $\theta$s along the path $\text{MKK}_\theta$ shown in Fig. 1(b). In panels (a,b) there is gap $\Delta$ in the spectrum at the Fermi level $\mu$. In panel (c) the spectrum is gapless and three bands cross the Fermi energy forming the Fermi surface. (d,e) The energy spectrum near the Dirac point $\text{K}$ calculated along the line parallel to $\Delta\text{K} = \text{K}_\theta - \text{K}$. (f) The Fermi surface calculated for $\theta = 1.89^\circ$ [panel (c)]. Different colors correspond to different bands intersecting the Fermi level. The black hexagon is the first Brillouin zone of the superlattice. The inset in (c) shows the four bands close to the Fermi level calculated along the line perpendicular to $\Delta\text{K}$ and crossing the Dirac point $\text{K}$ [the dot-dashed line in (f)].

surface with a non-zero density of states [see Fig. 2(f)]. With further decreasing $\theta$, the Fermi surface changes and may reduce to several Fermi points for definite set of the twist angles. Simultaneously, the density of states at the Fermi level oscillates with $\theta$. The accumulation of the density of states at zero energy was previously mentioned in Ref. [18].

Our calculations show that no gap exists between four low-energy bands and the lower or upper bands. Thus, the system remains metallic even when doped. On the other hand, the bands $E^{(\nu)}_k$ are quite flat if $\theta < \theta_c$; the Fermi velocities are about $10^{-3}$ times smaller than for a single graphene layer. Consequently, the disorder or the electron-electron interaction may qualitatively change the metallic band structure giving rise to localization or opening of a gap due to ordering.

To conclude, we study the tight binding model for the
tBLG. We demonstrate that at large twist angles it is an insulator. If \( \theta \) is below the critical angle, the tBLG may be a metal or a semimetal.

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