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Citation: Chin. Phys. B, 2021, 30 (**7**): 070311. DOI: 10.1088/1674-1056/ac00a3
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SPECIAL TOPIC — Twistronics

Projective representation of D_6 group in twisted bilayer graphene*

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(Received 12 May 2020; revised manuscript received 2 February 2021; accepted manuscript online 13 May 2021)

Within the framework of continuum model, we study the projective representation of emergent D_6 point group in twisted bilayer graphene. We then construct tight-binding models of the lowest bands without and with external electromagnetic fields, based on the projective representation.

Keywords: twisted bilayer graphene, tight-binding model, projective representation

PACS: 03.65.Fd, 71.20.−b, 71.23.An, 73.21.Cd **DOI:** 10.1088/1674-1056/ac00a3

1. Introduction

The recent experimental discovery of superconducting and strongly correlated insulating phases in the twisted bilayer graphene (TBG)[1–3] attracts tremendous attention and triggered massive theoretical studies.[4–22] TBG is a bilayer system in which two graphene layers are stacked to each other with rotational misalignment,[26–31] and the electronic band structure sensitively depends on the twist angle θ. Theoretically a small θ can produce a long-period moiré pattern, causing a severe folding of original bands and hence creating new low-energy bands in the moiré Brilluoin zone (MBZ),[32–44] especially when θ is near the so-called the magic angles.[39,41,43] Experimentally in TBG samples at θ near a magic angle of 1.05°, the insulating phase and the superconducting phase are observed around the filling of two electrons or holes per supercell.[1–3]

To understand the insulating and superconducting phases in TBG, one needs to construct Wannier orbitals and hence an effective tight-binding model for the lowest bands which are separated from the rest by energy gaps. We thus focus on the low-energy physics of TBG and neglect other details, which is captured by a long wave length model known as the continuum model of TBG.[42–44] In this work, we discuss the band structure of TBG within the framework of continuum model.

The low-energy band structure of TBG within the continuum model can be computed and turns out to depend on the twist angle. Near the magic angle, the band width is close to a local minimum, and the band symmetry has been studied intensively. Based on these band structure properties, some theoretical studies claim that Wannier orbitals of the lowest bands cannot be constructed to respect essential symmetries in TBG,[5,7,10] due to the so-called fragile topology.[22–24] While in some works of TBG, Wannier orbitals can be and have been constructed explicitly.[6–8]

In this work, we try to address on the Wannier orbital issue of TBG within continuum model, especially the appropriate representation of the symmetry group in the basis of these Wannier orbitals. We show that the Wannier orbitals constructed from the continuum model in Ref. [7] can furnish a projective representation of the point group, and the corresponding tight-binding model can reproduce the band structure of the lowest bands without fine tuning. To further test our construction, we apply external fields to TBG and show that the Wannier orbitals can also correctly describe the response to electromagnetic fields.

2. Projective representation of emergent D_6 group

We consider TBG on the long-range (superlattice constant $L_{\rm M} \sim 10$ nm) and low-energy (bandwidth of the lowest bands $\sim$10 meV) scales. Three special spots are found on the long range, namely, AA, AB, and BA spots, which are all centers for three-fold rotations, and AA is also the six-fold rotation center. The low-energy physics can be described by the continuum model, where both the emergent valley U(1) symmetry and D_6 point group symmetry are respected.

After successive symmetry operations $g_2, g_1 \in D_6$, the final operation is $g_1 g_2$ up to an U(1) phase ϕ

$$U(g_1)U(g_2) = \mathrm{e}^{\mathrm{i}\phi(g_1,g_2)\tau}U(g_1 g_2), \tag{1}$$

where U denotes the representation of D_6 and τ is the generator of valley U(1) symmetry. This type of representation of D_6 is known to be projective.

We then apply the projective representation of D_6 to Wannier orbitals of TBG within continuum model. We first consider TBG with atomic point group D_3 (Fig. 1(a)). From symmetry arguments, the Wannier orbitals of the lowest four

*Project supported by DOE Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-SC0010526.

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bands reside on the honeycomb lattice formed by AB and BA spots and have (p_x, p_y) on-site symmetry under D_3,[6] which have been constructed from atomic orbitals explicitly without U(1) symmetry.[8] Within the continuum model, the Wannier orbitals from individual valleys have also been constructed explicitly,[7] which we may call continuum model Wannier orbitals (CMWO). Two generators of D_6 are found in TBG: The in-plane six-fold rotation C_{6z} and out-of-plane two-fold rotation C_{2x}. When acting on CMWO, besides real-space operations, in momentum space C_{6z} will flip the valley index while C_{2x} will not, hence

$$U(C_{6z})|\boldsymbol{r},\tau\rangle = |C_{6z}\boldsymbol{r},-\tau\rangle, \tag{2}$$

$$U(C_{2x})|\boldsymbol{r},\tau\rangle = |C_{2x}\boldsymbol{r},\tau\rangle, \tag{3}$$

where $|\boldsymbol{r},\tau\rangle$ denotes CMWO at site $\boldsymbol{r}$ with valley $\tau = \pm$. From Ref. [7], we find that under C_{3z}, the CMWO with valley τ has angular momentum $-\tau$, namely,

$$U(C_{3z})|\boldsymbol{r},\tau\rangle = \mathrm{e}^{2\mathrm{i}\pi\tau/3}|C_{3z}\boldsymbol{r},\tau\rangle. \tag{4}$$

As $C_{3z} = C_{6z}^2$, to reconcile Eqs. (2) and (4), we must have $\phi(C_{6z}, C_{6z}) = 2\pi/3$. Other projective phases $\phi(g_1, g_2)$ can be worked out similarly. With nontrivial projective phases listed in Table. 1, we find that CMWO can furnish the projective representation of D_6 satisfying Eqs. (1)–(3), which incorporates the atomic representation of D_3. Under projective representation of D_6, CMWO can have s and $\mathrm{f} \equiv \mathrm{f}_{x(x^2-3y^2)}$ on-site symmetries, and $|\tau\rangle = |\mathrm{s}\rangle + \mathrm{i}\tau|\mathrm{f}\rangle$.

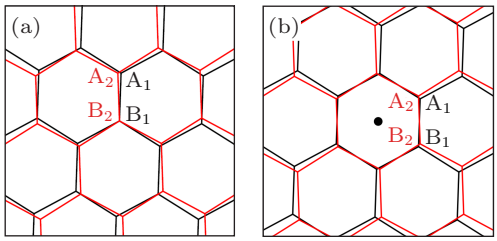


Fig. 1. Twisted bilayer graphene at $\theta = 1.05^\circ$ with atomic point groups (a) D_3 and (b) D_6. Black and red grids denote layers 1 and 2, A and B sublattices are also shown.

Table 1. The projective U(1) phase $\phi(g_1, g_2)$ of the projective representation in D_3 structure TBG, where $g_1, g_2 \in D_6$ are listed in rows and coloumns.

g_1	g_2						
	C_{6z}	C_{6z}^{-1}	C_{3z}	C_{3z}^{-1}	C_{2z}	C_{2y}	C_{2x}
C_{6z}	$\frac{2}{3}\pi$	0	$\frac{4}{3}\pi$	$\frac{2}{3}\pi$	$\frac{4}{3}\pi$	0	$\frac{4}{3}\pi$
C_{6z}^{-1}	0	$\frac{4}{3}\pi$	$\frac{4}{3}\pi$	$\frac{2}{3}\pi$	$\frac{2}{3}\pi$	0	$\frac{2}{3}\pi$
C_{3z}	$\frac{4}{3}\pi$	$\frac{4}{3}\pi$	0	0	$\frac{4}{3}\pi$	0	$\frac{4}{3}\pi$
C_{3z}^{-1}	$\frac{2}{3}\pi$	$\frac{2}{3}\pi$	0	0	$\frac{2}{3}\pi$	0	$\frac{2}{3}\pi$
C_{2z}	$\frac{4}{3}\pi$	$\frac{2}{3}\pi$	$\frac{4}{3}\pi$	$\frac{2}{3}\pi$	0	0	0
C_{2y}	0	0	0	0	0	0	0
C_{2x}	$\frac{4}{3}\pi$	$\frac{2}{3}\pi$	$\frac{4}{3}\pi$	$\frac{2}{3}\pi$	0	0	0

However, when we consider TBG with atomic point group D_6 (Fig. 1(b)), and adopt the atomic representation of D_6, the Wannier orbitals of the lowest four bands cannot be constructed from individual valleys.[5,7] This means that the atomic representation of D_6 is different from the projective representation of D_6 furnished by CMWO. In fact, the atomic representation of C_{2x} is different from its projective representation, hence if the atomic point group includes C_{2x}, then its atomic representation will not be compatible with the projective representation of D_6.

In terms of CMWO, we can write down the following tight-binding (TB) model of TBG:

$$H = \sum_{\tau=\pm}\sum_{ij} t(\boldsymbol{r}_{ij})\,\mathrm{e}^{\mathrm{i}\tau\varphi(\boldsymbol{r}_{ij})} c_{i\tau}^\dagger c_{j\tau}, \tag{5}$$

where $c_{i\tau}$ is the annihilation operator of CMWO at site i with valley τ, $\boldsymbol{r}_{ij}$ is the vector from site i to j, and $t(\boldsymbol{r}), \varphi(\boldsymbol{r})$ are the amplitude and phase of hopping integral along $\boldsymbol{r}$, respectively. The form of the TB model above manifests the time-reversal symmetry $\mathcal{T}$, and point group D_6 further restricts φ. For example, when we apply C_{6z} and $\mathcal{T}$, we find $\varphi(\boldsymbol{r}) = 0$ when $\boldsymbol{r} \parallel C_{6z}^n \hat{\boldsymbol{y}}$, $n = 0, 1, \ldots, 5$. Details of this TB model can be found in Ref. [7].

Due to projective representation, the emergent symmetry group of TB model Eq. (5) should be written as a semidirect product $D_6 \ltimes \mathrm{U}(1)$. To be complete, we can also include spin SU(2) and time reversal symmetry $\mathcal{T}$ and write the whole symmetry group in terms of both semidirect and direct products $D_6 \ltimes \mathrm{U}(1) \times \mathcal{T} \times \mathrm{SU}(2)$, which leads to an eight-fold Dirac point (including spin) at each K point of the moiré Brillouin zone.

When we break some symmetries and lower the symmetry group to its subgroup by external fields and other means, the band structure can be altered and the Dirac points at $\pm K$ points can be split. Such altered band structure can also be captured by the TB model in the basis of CMWO, which we will discuss in the following.

3. Responses to electromagnetic fields

As applications of CMWO and the effective TB model, we consider the band structure of TBG under electromagnetic fields.

An out-of-plane electric field will introduce an interlayer potential difference V. From the continuum model we can find that at each K point, V will split the eight-fold Dirac point into two four-fold Dirac points (spin included). As V breaks out-of-plabe rotation C_{2x} but preserves in-plane rotation C_{2z}, the Dirac points from individual valleys are protected by $C_{2z}\mathcal{T}$. The numerical results are shown in Fig. 2.

In the basis of CMWO, V furnishes A_2 representation of D_6 and is invariant under $\mathrm{U}(1) \times \mathrm{SU}(2) \times \mathcal{T}$, which we may call as a pseudo scalar. The linear response of the system to V can be described by the Hamiltonian $H_\mathrm{e} = V\mathcal{H}_\mathrm{e}$, and the invariance requires $\mathcal{H}_\mathrm{e}$ to have the same symmetry representation

as V, namely, a pseudo scalar furnishing A_2 representation of D_6 and invariant under U(1)×SU(2)×$\mathcal{T}$. One then searches for such pseudo scalars order by order in tight-binding (TB) framework. We find that the on-site and nearest-neighbor terms cannot be a pseudo scalar. Hence the leading order TB contribution of V is the next-nearest neighbor term

$$H_{\rm e} = g_{\rm e}\sum_{jn} {\rm i}\tau(-)^j c^{\dagger}_{j\tau}c_{j+\boldsymbol{L}_n,\tau}V + {\rm h.c.}, \tag{6}$$

where $\boldsymbol{L}_n = L_{\rm M}C^n_{3z}\hat{\boldsymbol{y}}$ $(n=0,1,2)$ are three bonding vectors of the next-nearest neighbors with superlattice constant $L_{\rm M}$, and $(-)^j = \pm$ for $j =$ AB and BA spots, respectively. The dimensionless coupling constant $g_{\rm e}$ depends on twist angle θ. We can add higher order TB terms (i.e., hopping at longer range) to improve our TB description of the electric field response.

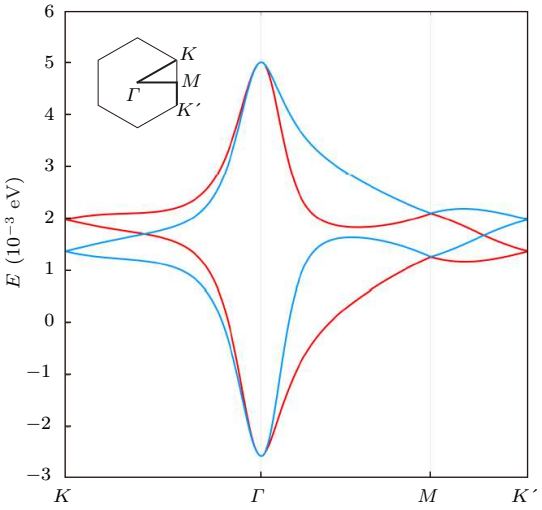


Fig. 2. Band structure of TBG $\theta = 1.05°$ with interlayer potential difference $V = 5$ meV based on continuum model, where blue and red lines are from valleys $\tau = \pm$, respectively. The moiré Brillouin zone and high symmetry lines (thick and black) for band structure are also shown at the left upper corner.

Another more subtle way to introduce an electric field is by substrates such as transition metal dichalcogenides or hexagonal boron nitrides, and the induced electric field will be highly nonuniform on atomic scale. In this case, the electric field can be captured by both interlayer potential difference V and sublattice potential difference V'.

Similarly, we find that V' furnishes B_1 representation of D_6 and is invariant under U(1)×SU(2)×$\mathcal{T}$. Hence the leading order TB contribution of V' is

$$H'_{\rm e} = g'_{\rm e}\sum_{jn} {\rm i}\tau c^{\dagger}_{j\tau}c_{j+\boldsymbol{L}_n,\tau}V' + {\rm h.c.}, \tag{7}$$

where dimensionless coupling constant $g'_{\rm e}$ also depends on twist angle θ.

Under an in-plane magnetic field $\boldsymbol{B}$, there will be orbital effect and spin effect. The spin effect is described by the on-site Zeeman term $H_{\rm s} = g_{\rm s}\sum_{\tau i}\mu_{\rm B}c^{\dagger}_{i\tau}\boldsymbol{\sigma}c_{i\tau}\cdot\boldsymbol{B}$, where $\mu_{\rm B}$ is the Bohr magneton and $g_{\rm s}$ is the spin g-factor. To describe the orbital effect, we choose vector potential $\boldsymbol{A}(z) = \boldsymbol{z}\times\boldsymbol{B}$ which only depends on out-of-plane coordinate $\boldsymbol{z} = (0,0,z)$. In this way, $\boldsymbol{B}$ does not break the translation symmetry, while breaks point group symmetries by introducing layer-dependent phases. As shown in Fig. 3, $\boldsymbol{B} = (B_x, 0)$ deforms the energy contours along x direction, breaking valley-preserving rotation C_{3z} and valley-flipping rotation C_{2y}. Valley-preserving rotation C_{2x} is preserved for $\boldsymbol{B}$ along high-symmetry x axis. For in-plane $\boldsymbol{B}$ not along high-symmetry directions, C_{2x} will also be broken.

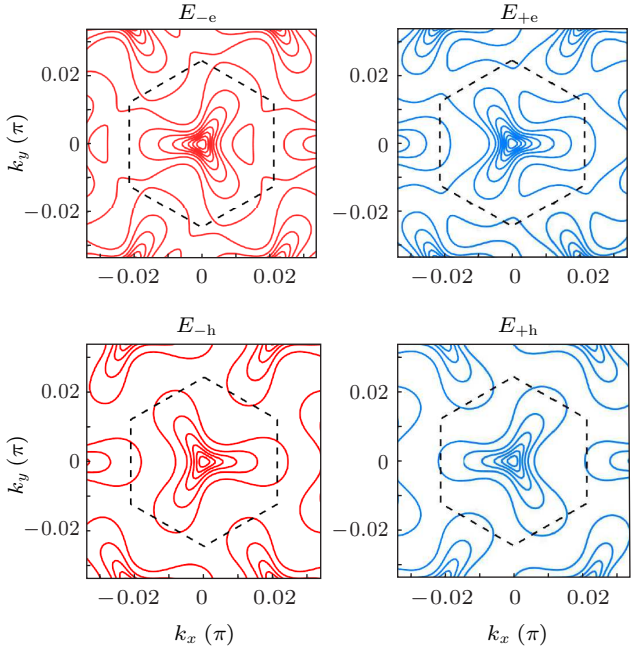


Fig. 3. Energy contours of the twisted bilayer graphene at $\theta = 1.05°$ with in-plane magnetic field $B = 1$ T along $\hat{\boldsymbol{x}}$ direction, based on continuum model. The blue and red lines denote bands from valley $\tau = \pm$, and e, h denote electron and hole sides, respectively.

In the basis of CMWO, $\boldsymbol{B}$ is a pseudo vector [E_1 representation of D_6, odd under $\mathcal{T}$ and invariant under U(1)×SU(2)]. Similarly, we search for TB terms which are pseudo vectors and find that unlike the spin effect, the on-site terms cannot be pseudo vectors. The leading order TB contribution of orbital magnetic field $\boldsymbol{B}$ is actually the nearest-neighbor term

$$H_{\rm m} = g_{\rm m}\mu_{\rm B}\sum_{\langle ij\rangle}(c^{\dagger}_{i+}c_{j+} - c^{\dagger}_{i-}c_{j-})\hat{\boldsymbol{e}}_{ij}\cdot\boldsymbol{B} + {\rm h.c.}, \tag{8}$$

where $\hat{\boldsymbol{e}}_{ij}$ is the unit vector from site i to j, and $g_{\rm m}$ is the dimensionless coupling constant analogous to spin g-factor. Similar to $g_{\rm e}(\theta)$, the dimensionless $g_{\rm m}$ is also a function of twist angle θ. Higher order TB terms at longer hopping ranges can be further included to improve our description of magnetic field response in TBG.

Within each valley, the TB term Eq. (8) describes the distortion of hopping integral along magnetic field direction, while the distrotions are opposite for opposite valleys. Thus we may regard the orbital field $\boldsymbol{B}$ as a valley-contrasting strain field, which distorts energy contours as shown in the continuum model and Fig. 3.

4. Conclusion

We show that Wannier orbitals can be constructed from each valley to furnish the projective representation of the point group D_6 in TBG within the framework of continuum model. Such Wannier orbitals and the corresponding tight-binding model can correctly describe the lowest bands without and with external magnetic fields.

Acknowledgement

We thank Liang Fu for important discussions.

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