Three-Dimensional Topological Twistronics

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We introduce a theoretical framework for the new concept of three-dimensional (3D) twistronics by developing a generalized Bloch band theory for 3D layered systems with a constant twist angle θ between successive layers. Our theory employs a nonsymmorphic symmetry that enables a precise definition of an effective out-of-plane crystal momentum, and also captures the in-plane moiré pattern formed between neighboring twisted layers. To demonstrate the novel topological physics that can be achieved through 3D twistronics, we present two examples including twisted graphite and twisted Weyl semimetals. In twisted graphite, Weyl nodes arise because of the inversion-symmetry breaking in the 3D twisted structure, with θ-tuned transitions from type-I to type-II Weyl fermions, as well as magic angles at which the in-plane velocity vanishes. In the second example of twisted Weyl semimetals, the moiré pattern associated with twisting induces a chiral gauge field $\mathcal{A}$ that has a vortex-antivortex lattice configuration. The vortex cores of the $\mathcal{A}$ field bind line modes with position dependent chiralities. By coupling these vortex line modes, moiré-scale Weyl physics emerges. We also discuss possible experimental realizations of 3D twistronics.

Introduction.— In a bilayer system with a small interlayer twist angle θ, moiré pattern forms and leads to novel two-dimensional (2D) phenomena. In twisted bilayer graphene (TBG), there are magic twist angles, at which Dirac Fermi velocity vanishes [1]. Low-energy bands become nearly flat and many-body interactions are effectively enhanced in TBG near the first magic angle, where superconducting and correlated insulating states have been experimentally observed [2, 3]. TBG represents a prototypical system for 2D twistronics [4], where the twist angle serves as a new tuning parameter. Given the greatly exciting 2D physics developing in TBG [5–14], it is natural to wonder whether the concept of twistronics can be generalized to 3D systems.

In this work, we introduce a general theoretical framework for 3D twistronics. Following the spirit of TBG, we consider a layered 3D structure shown in Fig. 1(a), where for every two adjacent 2D layers, the upper layer is rotated relative to the lower layer by a constant angle θ around a common out-of-plane axis. This twisted 3D structure breaks the translational symmetry in all spatial directions and thus the conventional Bloch theorem cannot be applied to analyze electronic structures. However, we establish the existence of an exact nonsymmorphic symmetry in this 3D twisted structure, which consists of an in-plane θ rotation followed by an out-of-plane translation. This screw rotational symmetry allows us to define a generalized Bloch theorem, where the modified crystal momenta are well defined. Our theory presents a general recipe for 3D twistronics, and various 3D moiré physics can be explored by simply considering different 2D building blocks as in Fig. 1(a).

With graphene as the 2D building block, we realize a twisted graphite model as a direct 3D generalization of TBG. Since the twisted structure intrinsically breaks inversion symmetry, we find that Weyl fermions appear abundantly in the twisted graphite. Moreover, the transition between type-I and type-II Weyl fermions can be induced by tuning the twist angle. We also establish the existence of two magic angles at which the in-plane Fermi velocity of the Weyl fermions vanishes, representing the first example of magic-angle Weyl physics.

The second example we consider is a twisted Weyl semimetal with a distorted lattice structure also shown in Fig. 1(a). The zero twist angle limit (θ = 0) of this model already hosts bulk Weyl nodes [15, 16], which is distinct from that of the twisted graphite. In a Weyl nanotube (the quasi 1D limit of our model), it is known that an externally applied torsion could result in chiral gauge fields that are minimally coupled to the low-energy Weyl fermions [17]. However, beyond the nanotube geometry, understanding the 3D bulk physics of a twisted Weyl semimetal remains an intriguing open question, which we solve in this work. In the 3D twisted Weyl semimetal, the emergent chiral gauge fields have a vortex-antivortex lattice configuration in the moiré pattern formed between two neighboring twisted layers. The vortex cores of the gauge fields bind line modes with position dependent chiralities. These line modes also wind around the screw rotational axis following the twisted lattice structure. The periodic array of the coupled vortex line modes realizes 3D Weyl nodes at the moiré scale, which provides a unique opportunity to manipulate the band structure of Weyl materials by changing the twist angle. Our work thus establishes the twist angle as an effective tuning parameter to study 3D Weyl physics.

Theory.— We construct a generalized Bloch band theory for generic 3D layered systems with a constant twist angle θ between successive layers [Fig. 1(a)]. The low-energy continuum Hamiltonian for this system is

$$H = \sum_n \int d^2 r \left\{ \psi_n^\dagger(r) h_n(k_\parallel) \psi_n(r) + |\psi_n^\dagger(r) T_n(r) \psi_{n+1}(r) + H.c. | \right\},$$

where $h_n(k_\parallel)$ is an effective out-of-plane crystal momentum, $T_n(r)$ is the effective twist angle, and $H.c.$ denotes the Hermitian conjugate. This Hamiltonian allows us to study the topological properties of 3D twistronics, including the emergence of Weyl fermions and the realization of moiré-scale Weyl physics. The transition between type-I and type-II Weyl fermions is induced by tuning the twist angle, providing a unique opportunity to manipulate the band structure of Weyl materials by changing the twist angle.
where $n$ is the layer index, $r$ and $k_{||}$ are respectively the 2D in-plane position and momentum, $\psi_k(r)$ represents the field operator for low-energy states, $h_n(k_{||})$ is the in-plane Hamiltonian for each 2D building block, and $T_n(r)$ is the interlayer tunneling. Here $\psi^\dagger$ can be a multicomponent spinor due to sublattices, orbitals, spins, etc. The layer dependence of $h_n$ and $T_n$ is determined by the twist relation:

$$h_n[\hat{R}(n\theta)k_{||}] = h_0(k_{||}), \quad T_n[\hat{R}(n\theta)r] = T_0(r),$$

where $\hat{R}$ is a rotation matrix. For small $\theta$, $T_0(r)$ has an in-plane moiré periodicity.

The 3D twisted structure generally breaks translational symmetry in all spatial directions, making it appear hopeless for theoretical treatments. However, Eq. (2) implies that the Hamiltonian $H$ is invariant under a nonsymmporphic operation, which rotates a layer by $\theta$ and then translates it along the out-of-plane $\hat{z}$ direction by the interlayer distance $d_z$. This nonsymmporphic symmetry suggests a generalized Bloch wave for the system:

$$\psi_{k_z}(r) = \frac{1}{\sqrt{N}} \sum_n e^{-ik_z r} \psi_n[\hat{R}(n\theta)r],$$

where $N$ is the number of layers, and the good quantum number $k_z$ is an effective out-of-plane crystal momentum measured in units of $1/d_z$. This Block wave is a superposition of electron states on a spiral line around the screw-rotation axis, as illustrated by the purple lines in Fig. 1(a). Under the generalized Bloch representation, Hamiltonian $H$ is

$$H = \sum_{k_z} \int d^2r \left\{ \psi_{k_z}^\dagger(r)h(k_{||})\psi_{k_z}(r) + \psi_{k_z}^\dagger(r)e^{ik_zT(r)}h(k_{||})\psi_{k_z}(r) + H.c. \right\},$$

where we use $h$ and $T$ as short-hand notations respectively for $h_0$ and $T_0$. It is worth noting that the appearance of $\hat{R}(\pm \theta)$ in Eq. (4) signals the breaking of in-plane translation symmetries. To proceed, we expand $T(r)$ by moiré harmonics: $T(r) = \sum g e^{i\theta g \cdot r}$, where $g$ is a moiré reciprocal lattice vector. $\hat{T}(r)$ generates in-plane momentum scatterings specified by $k'_{||} = \hat{R}(\theta)k_{||} + g$. For low-energy physics, the in-plane momentum $k_{||}$ is of the same order of magnitude as $g$, which is proportional to $\theta$. Thus, it is reasonable to approximate $\hat{R}(\pm \theta)$ by an identity matrix in the small $\theta$ limit. Under this approximation, $H$ acquires a moiré translational symmetry:

$$H \approx \sum_{k_z} \int d^2r \psi_{k_z}^\dagger(r)\left[ h(k_{||}) + \Delta(k_z, r) \right] \psi_{k_z}(r),$$

$$\Delta(k_z, r) = e^{ik_zT(r)} + e^{-ik_zT^\dagger(r)},$$

which gives rise to band structure in the 3D momentum space spanned by $k_z$ and the in-plane moiré Brillouin zone. Eq. (5) is our effective Hamiltonian for the 3D small-angle twisted system, which builds in exactly the nonsymmporphic symmetry and captures the moiré pattern formed in neighboring twisted layers.

**Twisted Graphite.**— We apply our theory to study electronic structure of twisted graphite, which we construct by starting from an infinite number of graphene layers with $AAA...$ stacking, and then rotating the $n$th
layer by $n\theta$ around a common hexagonal center. In each layer, low-energy electrons reside in $\pm K$ valleys, which are related by spinless time-reversal symmetry $\hat{T}$ and can be studied separately as in TBG. We focus on $+K$ valley, with the in-plane $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian $h(k) = \hbar v_F k \cdot \sigma$, where $v_F$ is the monolayer graphene Dirac velocity ($\sim 10^6$ m/s) and $\sigma$ is the sublattice Pauli matrix. The interlayer tunneling $T(r)$ is

$$T(r) = \sum_{j=0,1,2} \left( \begin{array}{cc} w_{AA} & w_{AB} e^{-i2\pi j/3} \\ w_{AB} e^{i2\pi j/3} & w_{AA} \end{array} \right) e^{i\ell_z r}$$

where $w_{AA}$ and $w_{AB}$ are respectively intra-sublattice and inter-sublattice tunneling parameters, with $w_{AA} \approx 90$ meV and $w_{AB} \approx 117$ meV. $g_j$ is a moiré reciprocal lattice vector $(0, 4\pi/3a_M)$, and $a_M = a_0/\theta$, where $a_0$ is the monolayer graphene lattice constant. The other two vectors $g_{2,3}$ are related to $g_1$ by $\pm 2\pi/3$ rotations. We note that $a_M$ is the TBG moiré periodicity, but $T(r)$ in Eq. (6) has a periodicity of $a_M = \sqrt{3}a_M$.

The $k_z$-dependent moiré potential $\Delta = e^{i\ell_z} T + e^{-i\ell_z} T^\dagger$ can be decomposed into $\Delta_0 \sigma_0 + \Delta_x \sigma_x + \Delta_y \sigma_y$, where $\Delta_0$ is a scalar potential. From $\Delta$, we can define an effective gauge field $\mathbf{A} = (\Delta_x, \Delta_y)/(ev_F)$ that couples to the Dirac Hamiltonian $h(k)$, and a corresponding pseudo magnetic field $b_z = \nabla \times \mathbf{A}$. 2D maps of $\Delta_0$ and $b_z$ at $k_z = 0$ are plotted in Fig. 2(c), which shows that $|b_z|$ can reach $\sim 200$ T for $\theta = 1.1^\circ$.

The effective Hamiltonian $\mathcal{H} = h(k) + \Delta$ respects $\hat{C}_3z$ and $\hat{C}_2z\hat{T}$ symmetries, where $\hat{C}_nz$ is a $n$-fold rotation around $\hat{z}$ axis. In addition, $\mathcal{H}$ has two emergent symmetries: (1) a translation like symmetry $\mathcal{H}(k, k + 2\pi/3, r + a_M \hat{y}) = \mathcal{H}(k, k, r)$, which makes energy spectra at $k_z$ and $k_z + 2\pi/3$ identical and also guarantees physical quantities such as electron density to have a period of $a_M$ instead of $a_M$; (2) a particle-hole like symmetry $\mathcal{H}(-k, -k_z, -r) = -\mathcal{H}(k, k_z, r)$.

We diagonalize $\mathcal{H}$ using a plane-wave expansion, and show the calculated band structures at $\theta = 1.1^\circ$ in Figs. 2(a) and 2(b). Bands along $k_z$ axis can be characterized by the $\hat{C}_nz$ angular momentum $\ell_z \in \{0, \pm 1\}$. As shown in Fig. 2(a), crossings between two bands with different $\ell_z$ actually represent 3D Weyl nodes, which appear abundantly along $k_z$ axis. For example, the Weyl fermion at $\gamma$ point ($k = 0$) has an effective Hamiltonian $\mathcal{H}(v_F^+ k_{\parallel} \cdot \sigma + v_F^+ k_z \sigma_z)$, which is constrained by both $\hat{C}_3z$ and $\hat{C}_2z\hat{T}$ symmetries. The $\theta$ dependence of $(v_F^+, v_F^+)$ is shown in Fig. 2(c). $v_F^+$ is reduced from the bare value $v_F$, but remains finite for $\theta$ from $0.7^\circ$ to $2^\circ$. Remarkably, the sign of $v_F^+$ oscillates with $\theta$, and therefore, the chirality of the Weyl node at $\gamma$ point is twist angle dependent.
Another representative Weyl node is located at $k_{1/2} = (0, 0, \pi/2)$. This Weyl node is pinned to zero energy by the particle-hole like symmetry, and is described by $h[\sigma + v_1 q_z (\sigma_0 + \sigma_2)/2 + v_2 q_x (\sigma_0 - \sigma_2)/2]$, where $v_{1,2}$ are two independent parameters and $q_z = k_z - \pi/2$. For $\theta$ between $1^\circ$ and $1.8^\circ$, $v_2$ is always negative, but $v_1$ changes sign at $\theta_{1,1} \approx 1.52^\circ$ and $\theta_{2,2} \approx 1.22^\circ$, which are critical angles that mark transitions between type-I and type-II Weyl fermions [Fig. 1(b)]. Moreover, the in-plane velocity $v_1$ vanishes at both $\theta_{M,1} \approx 1.67^\circ$ and $\theta_{M,2} \approx 1.09^\circ$, which can be identified as two magic angles. Here the value of $\theta_{M,1}$ can also be estimated using an analytical perturbation theory, agreeing quantitatively with our direct band structure calculations. The low-energy density of states (DOS) per layer in the 3D twisted graphite near the magic angles is orders of magnitude larger than that in monolayer graphene [Fig. 2(d)], which should enhance interaction effects, leading to interaction driven quantum phase transitions.

We now compare our results with related works. Ref. [19] studied multiple graphene layers with twist angle $(-1)^n \theta$ that alternates with the layer index $n$. Their 3D structure preserves inversion symmetry, in contrast with our twisted graphite structure shown in Fig. 1(a). Ref. [20] studied the same structure as ours but with a different method under the coherent phase approximation. Our theory employs the exact nonsymmorphic symmetry, which allows us to precisely define the $k_z$ momentum and clearly demonstrate magic-angle Weyl physics in twisted graphite. In Ref. [21], twisted trilayer graphene has been theoretically studied. An interesting question is how many layers are required in practice to realize our predicted 3D physics of twisted graphite, which we leave for future study.

**Twisted Weyl Semimetal.** — As another demonstration, we apply our theory to twisted Weyl semimetals with lattice structure also shown in Fig. 1(a). We start by introducing a minimal Weyl semimetal model on a simple cubic lattice (lattice constant $a_0$): $h_W = \hbar v_W k_\parallel \cdot \sigma + M(k) \sigma_z$, where $M(k) = M_0 (\cos k_z - \cos Q_x) - M_1 k_2$ with parameters $M_{0,1} > 0$ and $0 < Q_x < \pi$. Each site on the cubic lattice accommodates two orbitals $|j_z = \pm 1/2\rangle$ with different angular momentum $j_z$ and form the basis of the Pauli matrices $\sigma$. The Hamiltonian $h_W$ breaks time reversal symmetry and hosts two Weyl nodes with opposite chiralities located respectively
at \( k_z = (0, 0, \pm Q_z) \).

We now consider a twisted cubic lattice in which the \( n \)th layer is rotated by \( n\theta \) around the \( z \) axis following Fig. 1(a). The effective Hamiltonian \( \mathcal{H}_W \) for this twisted structure is given by

\[
\mathcal{H}_W = h_W + 2t_{sp} \sin k_z \sum_g \left( \begin{array}{cc} 0 & e^{i(g_y + g_z)} \\ e^{-i(g_y + g_z)} & 0 \end{array} \right)
\]

where \( t_{sp} \) characterizes the inter-orbital tunneling between neighboring layers. The summation over \( g \) is restricted to the first shell of moiré reciprocal lattice vectors \( \{g\} = 2\pi/a_M \) with moiré period \( a_M = a_0/\theta \), and \( g_y \) is the orientation angle of \( g \). Here the interlayer tunneling matrix is derived using a two-center approximation [11], and we neglect the spatial modulation of interlayer intra-orbital tunneling. Compared with the twisted graphite Hamiltonian, \( \mathcal{H}_W \) does not have a scalar moiré potential term.

We can extract an effective gauge field \( \mathbf{A} \) from \( \mathcal{H}_W \), similar to the case of twisted graphite. The \( \mathbf{A} \) field has a vortex-antivortex lattice configuration in the moiré superlattices. The corresponding pseudo magnetic field \( b_z \) is given by

\[
b_z = \frac{2t_{sp}}{e v_W a_M} \sin k_z \sum_g e^{i g_y + g_z},
\]

which is illustrated in Fig. 3(b). \( |b_z| \) peaks at two distinct types of positions in the moiré pattern, namely, integer positions \( \mathcal{R} = (n_x, n_y) a_M \) with \( n_{x,y} \in \mathbb{Z} \) and half-integer positions \( \mathcal{R}_{1/2} = \mathcal{R} + (\frac{1}{2}, \frac{1}{2}) a_M \), which are also locations of vortex cores of the \( \mathbf{A} \) field. We assume \( t_{sp}/v_W > 0 \), and \( b_z \) is positive and negative respectively at \( \mathcal{R} \) and \( \mathcal{R}_{1/2} \) for \( 0 < k_z < \pi \). Being proportional to \( \sin k_z \), \( b_z \) represents a chiral magnetic field as it couples oppositely to the Weyl nodes with different topological charges. In the semiclassical picture, around \( \mathcal{R} (\mathcal{R}_{1/2}) \) positions, this chiral magnetic field leads to chiral Landau levels that propagate along positive (negative) \( z \) direction for both Weyl nodes at \( k_z \). These chiral Landau levels bound to vortex cores of the \( \mathbf{A} \) field can be considered to be vortex line modes (VLMs). The chirality of a VLM depends on its position in the moiré pattern. An important physical consequence is that an out-of-plane electric field can drive a real-space pumping of electrons from \( \mathcal{R} \) to \( \mathcal{R}_{1/2} \) positions, or vice versa. The 2D array of VLMs can further hybridize with each other, and we expect them to realize Weyl fermions with moiré-scale modulations in the wave functions.

To verify the above picture, we numerically diagonalize \( \mathcal{H}_W \), and show the energy spectrum along \( k_z \) in Fig. 3(a), where we find that the Weyl nodes are robust against the twist. In Fig. 3(d) [Fig. 3(e)], we plot the real-space probability density of the right (left) moving modes highlighted in Fig. 3(a), which is found to be primarily concentrated at \( \mathcal{R} (\mathcal{R}_{1/2}) \) positions. This density profile is consistent with the above semiclassical analysis. Because of the twisted structure, these modes track spiral lines in real space. From the semiclassical picture, the in-plane velocity \( v_W^* \) of the 3D Weyl fermions is controlled by the coupling strength between neighboring VLMs, and therefore, by the moiré period \( a_M \). Numerical results plotted in Fig. 3(c) confirm that \( v_W^* \) decreases with decreasing \( \theta \) (equivalently, increasing \( a_M \)). For small enough \( \theta \), \( v_W^* \) nearly vanishes, showing that VLMs located at different positions are essentially decoupled. Thus, the twist angle provides a new tuning knob to control the band structure of 3D Weyl materials.

Conclusion.— In summary, we develop a general theoretical framework of 3D twistronics and present two examples, i.e., twisted graphite and twisted Weyl semimetal. In principle, one can take other 2D materials, e.g., \( AB \) bilayer graphene and \( ABC \) trilayer graphene, as the building block in Fig. 1(a) to study various 3D twistronics systems using our recipe.

In addition to solid state materials, our theory can also be realized in photonic systems. Recent experiments have demonstrated both 3D Weyl physics and 2D graphene-related topological physics in photonic waveguides [22], gyroids [23], metamaterials [24], and magnetized semiconductors [25]. Strain-induced gauge field effects have also been engineered in Weyl metamaterials [29]. The flexibility of building photonic lattices makes them an ideal platform for our proposed 3D topological twistronics.

One appealing feature of TBG twistronics is the strong enhancement of 2D correlation effects tuned by the twist angle. The two models studied in this work provide new playgrounds for strongly correlated Weyl physics in 3D. As an example, superconductivity can occur in 3D twisted graphite near the magic angles due to the strong velocity suppression.

Acknowledgment.— We thank Yang-Zhi Chou for discussions. This work is supported by Laboratory for Physical Sciences and Microsoft. R.-X. Z. is supported by a JQI Postdoctoral Fellowship.

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