Discovery of High Dimensional Band Topology in Twisted Bilayer Graphene

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Abstract:
Recently twisted bilayer graphene(t-BLG)¹-⁵ emerges as a new strongly correlated physical platform near a magic twist angle⁴, which hosts many exciting phenomena such as the Mott-like insulating and unconventional superconducting behavior⁶-¹⁰. Besides the apparent significance of band flatness⁴, band topology may be another critical element in strongly correlated twistrronics yet receives much less attention¹¹-¹⁴. Here we report the discovery of nontrivial high dimensional band topology in t-BLG moiré bands through a systematic nonlocal transport study¹⁵, ¹⁶, in conjunction with an examination rooted in K-theory¹⁷. The moiré band topology of t-BLG manifests itself as two pronounced nonlocal responses in the electron and hole superlattice gaps. We further show that the nonlocal responses are robust to the interlayer electric field, twist angle, and edge termination, exhibiting a universal scaling law. While an unusual symmetry of t-BLG trivializes Berry curvature, we elucidate that two high dimensional Z² invariants characterize the topology of the moiré Dirac bands, validating the topological origin of the observed nonlocal responses. Our findings not only provide a new perspective for understanding the emerging strongly correlated phenomena in twisted van der Waals heterostructures, but also suggest a potential strategy to achieve topologically nontrivial metamaterials from topologically trivial quantum materials based on twist engineering.

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It is widely known that overlaying two identical periodic lattices with a relative twist generates a larger-scale interference structure, i.e., the moiré pattern. For two-dimensional (2D) materials, such twists create moiré superlattices by reducing translation symmetry in real space and folds electron Bloch bands into moiré Brillouin zones (MBZ) in momentum space\textsuperscript{1-5}. The moiré bands can exhibit striking phenomena such as the Hofstadter’s butterfly in fractal quantum Hall effect\textsuperscript{18-20} and the moiré potential-modulated interlayer excitons\textsuperscript{21-24}. Remarkably, strongly correlated electron behavior including Mott-like insulating phases and possibly unconventional superconductivity have been discovered in twisted bilayer graphene (t-BLG) near a magic angle\textsuperscript{4} (\textasciitilde1.1°) and in aligned trilayer graphene/hexagonal boron nitride (hBN) heterostructures\textsuperscript{25, 26}. Besides their extreme band flatness, nontrivial band topology may be another crucial feature in determining the observed strongly correlated phases. One celebrated example is the well-studied incompressible fractional quantum Hall effect\textsuperscript{11}, in which the partially filled Landau level has a nontrivial Chern number\textsuperscript{12}. Another example is the predicted \(Z_4\) parafermions\textsuperscript{13}, for which the 8\(\pi\) Josephson effect is mediated by a helical edge state of 2D topological insulator (TI)\textsuperscript{14} with a sufficiently small velocity. Therefore, it is of significance to investigate the possible topology of the active moiré bands in these correlated systems, which however has yet to be demonstrated experimentally, despite the most recent tantalizing discussions relating the t-BLG band topology to the concept of wannierizibility\textsuperscript{27-29}.

Here we experimentally reveal the universal and unique moiré band topology of t-BLG at small twist angles by using systematic nonlocal transport measurements\textsuperscript{15, 16, 30-32}. Previously, a nonlocal measurement scheme has been employed in detecting the helical edge state of 2D TI\textsuperscript{15} and the topological valley current driven by Berry curvature\textsuperscript{16, 30-32}. In this work, pronounced nonlocal responses are observed in both the electron and hole superlattice gaps of t-BLG\textsuperscript{33} and persist in a wide range of applied displacement fields from 0 to 0.62 V/nm. Moreover, the nonlocal responses are consistently observed in 15 t-BLG devices with twist angles between \textasciitilde1.3° and \textasciitilde1.9°, showing their robustness to twist angle and edge termination. We elucidate that the unique \(C_2zT\) symmetry of t-BLG, though trivializing any Berry curvature, gives rise to two nontrivial bulk \(Z_2\) invariants that previously appear in six and seven dimensions in the celebrated periodic table of topological classification\textsuperscript{17}. While one invariant protects the moiré Dirac points, the other dictates
the presence of one pair of counter-propagating edge states per spin-valley in each superlattice gap. We further show that the observed non quantization and universal scaling of nonlocal resistance are consistent with the $C_{2z}T$ and valley symmetry breaking at edges. Our findings not only unveil the appealing moiré band topology of t-BLG but also offer a universal pathway for creating topological metamaterials by twist engineering 2D materials. The discovered moiré band topology may provide a new perspective for deciphering the tantalizing strongly correlated phenomena$^6$-$^10$ in magic-angle t-BLG.

A schematic of our typical t-BLG devices is shown in Fig. 1a. We employed a “tear-and-stack” technique to fabricate hBN encapsulated t-BLG heterostructures as reported previously$^5,33,34$ (Methods). A Hall-bar geometry was defined through reactive ion etching, and electrical contacts to t-BLG were made at the edge$^{34}$. The total carrier concentration $n$ in t-BLG, estimated based on a capacitor model, is controlled by tuning the voltage applied to the global silicon back gate. The schemes of local and nonlocal measurements are illustrated in the lower inset in Fig. 1b. We first characterize the t-BLG moiré superlattice by measuring the four-probe local resistance $R_L$ as a function of $n$ at 80 K in a device (D1) shown in the top inset in Fig. 1b. (See Extended Data Fig. 1a for the complete temperature dependence of $R_L$ down to 10 K.)

Three resistance maxima are observed at the charge neutrality point and at $n = \pm n_s \approx 6.50 \times 10^{12}\text{cm}^{-2}$ (Fig. 1b), at which the Fermi level crosses the degenerate Dirac points from the two original graphene monolayers and the two moiré superlattice-induced band gaps due to the interlayer hybridizations$^{33}$, respectively. Here, $n_s$ denotes the carrier concentration corresponding to 4 electrons per moiré unit cell$^{33}$, from which we can deduce the twist angle of this device to be $\sim1.68^\circ$. The error is estimated to be around $\pm0.05^\circ$. Figure 1c shows the calculated moiré band structure of $1.68^\circ$ t-BLG (Methods), where the red region in the middle and the two white regions adjacent to it highlight the two moiré Dirac bands (per spin-valley) and the two superlattice gaps, respectively. Both of the superlattice gaps are extracted to be $\sim40$ meV based on the temperature dependent transport measurements (Extended Data Fig. 1b), which is slightly larger than the calculated gaps (Fig. 1c). Strikingly, pronounced nonlocal responses $R_{NL} = V/I$ are observed in
the superlattice gaps on both the electron- and hole-sides, as featured in Fig. 1b. The peaks of $R_{NL}$ have a narrower range in $n$ compared with that of $R_L$ and attenuate to zero away from $\pm n_s$.

We first exclude the possibility from stray current-induced Ohmic nonlocal resistance, which can be estimated by the van der Pauw relation \( R_{NL,Ohmic} = R_L w / \pi L \exp(-\pi L/w) \). Here $L = 3 \mu m$ is the channel length between the driving and probing terminals and $w = 1.2 \mu m$ is the channel width. The Ohmic contribution only yields $R_{NL,Ohmic} < 1 \Omega$ at the superlattice gaps, which is at least two orders of magnitude smaller than our observed $R_{NL}$ peak values. With lowering the temperature to 1.7 K, $R_{NL}$ continues to grow and exhibits fluctuations without any obvious quantization (Extended Data Fig. 2). While excluding the presence of protected gapless edge states\cite{15}, our observation is reminiscent of the nonlocal transport driven by valence-band Berry curvatures\cite{39} in several 2D materials\cite{16,30-32}. However, Berry curvature vanishes in t-BLG. The $C_{2z}$ rotational symmetry requires the Berry curvatures of opposite momenta to be the same, whereas the time-reversal ($T$) symmetry requires them to be opposite. Thus, the $C_{2z}T$ symmetry of t-BLG leaves any momentum invariant and dictates any Berry curvature to be zero.

Because $(C_{2z}T)H(k)(C_{2z}T)^{-1} = H(k)$ and $(C_{2z}T)^2 = 1$, t-BLG Hamiltonian $H(k)$ belongs to class AI in the celebrated periodic table of topological classification rooted in $K$-theory\cite{17}. In this classification (Table 1), the topological invariant of $H(k)$ is determined by $d$-$D$, where $d$ ($D$) denotes the number of dimensions in which momentum is odd (even) under $C_{2z}$-$T$. Evidently, t-BLG can be characterized by two independent $Z_2$ invariants, as $H(k)$ is featured by $d=0$ and $D=1$ or 2. We find that both invariants are nontrivial for the moiré Dirac bands of t-BLG (per spin-valley). One $Z_2$ invariant ($d$-$D=7$ in Table 1) amounts to the quantized Berry phase ($0$ or $\pi$) of the lower band along a loop in the MBZ. The $\pi$ Berry phase ensures the presence of Dirac points at $K_s$ or $K'_s$ in the MBZ, which is confirmed by our observation of minimum conductivity at the charge neutrality below $\sim 60$ K (Extended Data Fig. 1a) and previous measurements by other groups\cite{33,40}.
Table 1. Topological classification\textsuperscript{17} for class AI in the Altland-Zirnbauer table. The cases with $d = 0$ and $D = 1, 2$ are relevant for the moiré Dirac bands of t-BLG. Because of the unique $C_{2z}T$ symmetry, the nontrivial $Z_2$ index of $d-D = 7$ protects each bulk Dirac point, and the nontrivial $Z_2$ index of $d-D = 6$ (Fig. 1e) leads to the (gapped) counter-propagating edge states in each superlattice gap (Fig. 1f).

The other $Z_2$ invariant ($d-D=6$ in Table 1) over the entire MBZ can be visualized by computing the Wilson loop spectral flow\textsuperscript{41} of the two moiré Dirac bands. This spectral flow corresponds to a wannier-center counterflow (calculated by using circle 1 in Fig. 1d) along a loop (circle 2 in Fig. 1d) around the MBZ (torus in Fig. 1d), and the $Z_2$ invariant characterizes the parity of the counterflow winding. In Fig. 1e, the red traces illustrate the counterflow winding for the two moiré Dirac bands, and the two crossings are symmetry-enforced stable points (Methods). Consistent topological features have also been discussed\textsuperscript{27-29}, based on different and complicated approaches. The nontrivial counterflow, reminiscent of that of 2D TI\textsuperscript{41}, implies the presence of a pair of counter-propagating edge states per spin-valley in the electron superlattice gap (dashed curves in Fig. 1f). Because of the particle-hole symmetry evidenced in Fig. 1c, such edge states also exist in the hole superlattice gap. Yet, due to the breaking of $C_{2z}T$ and valley symmetries by t-BLG boundary, the edge states acquire gaps (solid curves in Fig. 1f). This is consistent with our observation of non-quantized nonlocal responses at low temperatures; the spreading of edge states into the bulk forms quasi-one-dimensional diffusion channels.

Next, we examine the impact of interlayer electric field on the discovered nonlocal response. To independently control the total carrier concentration $n$ and the average displacement field $D$, we fabricated a dual-gate t-BLG device (D2). In this device (inset in Fig. 2a), by tuning the top ($V_{TG}$) and bottom ($V_{BG}$) gate biases, we achieve $n = -(C_{TG}(V_{TG} - V_{TG,0}) + C_{BG}(V_{BG} - V_{BG,0}))/e$ and $D = (-C_{TG}(V_{TG} - V_{TG,0}) + C_{BG}(V_{BG} - V_{BG,0}))/2\varepsilon_0$ based on a parallel-capacitor model\textsuperscript{42}. Here $\varepsilon_0$ is the vacuum permittivity, $e$ is the electron charge, $C_{TG}$ ($C_{BG}$) is the capacitance of top (back)
gate-dielectric layer, and $V_{TG,0}$ ($V_{BG,0}$) is the offset voltage due to unintentional doping. In Fig. 2a we show the local resistance $R_L$ mapping as a function of both $V_{TG}$ and $V_{BG}$ at 80 K. The two superlattice gaps manifest as the resistance maxima along the constant doping lines $n = \pm n_s$. As $|D|$ changes from 0 to 0.62 V/nm, $R_L$ at $n_s$ ($-n_s$) varies by a factor of $\approx 1.5$ (2.5). The moderate change in $R_L$ implies that the superlattice gaps are not closed by the applied $D$ fields. Consistently, the calculated moiré bands do not exhibit any qualitative change for an interlayer potential difference of 100 meV (Extended Data Fig. 3).

Importantly, as shown in Fig. 2b, appreciable nonlocal responses are observed at $n = \pm n_s$ no matter whether or not the $D$ field vanishes. ($R_{NL}$ drops dramatically to zero away from $\pm n_s$.) Not only is this consistent with the fact that the $D$ field does not break the $C_{2z}$ symmetry, it also validates that the origin of nonlocal responses in t-BLG is distinct from the electric field driven Berry curvatures in other 2D materials. On the electron side, the $R_{NL}$ peak decreases from $\approx 1.4$ to $\approx 0.9$ kΩ as $D$ reduces from 0.62 to 0.02 V/nm (Fig. 2b). We attribute the moderate enhancement in $R_{NL}$ with $D$ to the possible formation of network of AB-BA domain wall modes under $D$ fields. Such a conducting network has been imaged in t-BLG and may contribute to the nonlocal transport. The nonlocal responses on the hole side exhibit a relatively complex dependence on $D$ for $D < 0$. Sharp negative $R_{NL}$ peaks appear on the higher concentration side as $D$ increases from $-0.3$ V/nm to 0. (See Methods for detailed discussions on the hole-side $R_{NL}$.) The imperfect particle-hole symmetry of t-BLG may explain the observed asymmetric $D$ dependence of $R_{NL}$ on the electron and hole sides. Nevertheless, similar particle-hole asymmetry has also been noticed in other t-BLG studies.

We now extend our nonlocal measurements to t-BLG of different twist angles. We observe that the nonlocal responses are universal in all our t-BLG devices with twist angles from $\approx 1.3^\circ$ to $\approx 1.9^\circ$. Figure 3 denotes the nonlocal measurement results from Devices 3 to 7. (See Extended Data Table 1 for the device details.) For each twist angle, the red curve plots the measured $R_{NL}$ data recorded at 80 K, whereas the blue curve plots the calculated density of states (DOS) as a function of carrier concentration $n$ (Methods). For each twist angle, the pronounced $R_{NL}$ peaks coincide well with the
DOS minima, which correspond to the two superlattice gaps separating the moiré Dirac bands in t-BLG spectra. We emphasize that the moiré Dirac bands of our studied small-angle t-BLG are topologically equivalent since the superlattice gaps do not close as the twist angle decrease from ~2° to the magic angle ~1.1° (Methods and Extended Data Fig. 3). Thus, our observation above the magic angle reveals unambiguously the nontrivial band topology of the moiré Dirac bands as a whole near the magic angle. Moreover, the standard etching process (Methods) defined arbitrary edge terminations in our devices. Thus, the existence of strong nonlocal responses in all our t-BLG devices implies the robustness of the observed phenomenon against the edge termination.

To further elaborate the physical mechanism of the observed nonlocal responses, we measure the length dependence of $R_{NL}$ in a multi-terminal Hall bar device (D8) at 80 K. From the local resistance measurement, we estimate that the twisted angle is ~1.89°. Figure 4a displays three set of $R_{NL}$ data obtained by choosing three channels with different driving and/or probing terminal pairs, as illustrated by the device micrograph in the upper inset in Fig. 4a. We notice that the peak positions of different channels are slightly off aligned, which is likely due to the charge inhomogeneity in the sample. Quantitatively, the $R_{NL}$ peak values exponentially decay with the channel length $L$ (lower inset in Fig. 4a), and the linear fitting in the semi-log plot yields characteristic diffusion lengths $\lambda_e \approx 1.2 \, \mu m$ and $\lambda_h \approx 1.4 \, \mu m$ for the electron- and hole-side, respectively.

The scaling between $R_{NL}$ and $R_L$ is essential to understand the nonlocal transport mechanism. A power-law relation $R_{NL} \sim R_L^\alpha$ is revealed by the Arrhenius plot (Fig. 4b) for the data points around $R_{NL}(R_L)$ peaks in the range $n \pm \Delta n = -5.54 \pm 0.28$ and $5.54 \pm 0.22 \, (10^{12} \, \text{cm}^{-2})$ measured in a 1.54° t-BLG device (D9). The fitting parameter $\alpha$ is found to be 3.00 (2.51), 3.37 (2.36), 3.01 (2.17) and 3.50 (2.29) for hole-side (electron-side) responses at 80, 90, 100, and 110 K, respectively. This power-law scaling, together with the above revealed diffusion behavior, suggests that $R_{NL} \sim R_L^\alpha e^{-L/\lambda}$. Furthermore, the magnitude of $R_{NL}$ peaks on both electron and hole sides are reduced by ~100 times from 80 to 180 K (Fig. 4c). At room temperature, the nonlocal responses can no longer be clearly identified. From the semi-log plot of $R_{NL}$ peak versus $1/T$ (inset...
in Fig. 4c), it is clear that $R_{NL}$ has similar thermal activation behavior as $R_L$ in the superlattice gaps. The activation energies $E_{NL}$ ($E_L$) are extracted to be $157 \pm 20$ meV ($36 \pm 1$ meV) and $129 \pm 16$ meV ($34 \pm 2$ meV) for the electron and hole sides, respectively, with $E_{NL}/E_L \sim 4$. We attribute this deviation from $\alpha$ to the temperature dependence of $\lambda$, since stronger scattering at higher temperature reduces $\lambda$ and effectively enhances $E_{NL}/E_L$.

The observed scaling relation between $R_{NL}$ and $R_L$ in t-BLG is rather unusual. Previously, similar behavior is suggested for the spin Hall effect\cite{49} and seen for the valley Hall effects\cite{16, 30-32}, where the nonlocal transport is captured by a cubic law $R_{NL} \sim R_L^2 \sigma_{xy}^{\nu,s} e^{-L/\lambda^{\nu,s}/\lambda^{\nu,s}}$. Here $\sigma_{xy}^{\nu,s}$ and $\lambda^{\nu,s}$ refer to the valley (spin) Hall conductivity and the valley (spin) diffusion length, respectively. In t-BLG, the symmetry-trivialized Berry curvature and negligibly weak spin-orbit coupling imply vanishing $\sigma_{xy}^{\nu,s}$. However, the spreading of gapped edge states into the bulk forms quasi-one-dimensional diffusion channels and support the nonlocal transport over 1 μm at 80 K. Future measurements through scanning tunneling microscope\cite{40, 48}, scanning superconducting quantum interference\cite{50, 51}, and microwave impedance microscopy\cite{52} may directly image such edge channels in the t-BLG superlattice gaps. Nevertheless, the robustness of observed nonlocal signatures against the interlayer electric field, twist angle, and edge termination not only provides compelling evidence for the nontrivial band topology of t-BLG but also may open a new avenue for creating, engineering, and exploiting moiré quantum information by twistronics and nonlocal means.

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Figure captions

Figure 1 | Signature of band topology in small-twist-angle bilayer graphene. a, Schematic of a typical single-gate device with t-BLG channel. The carrier concentration \( n \) is tuned by a global silicon back gate. Inset: Schematic moiré pattern of t-BLG consisting two layers of monolayer graphene with a twist. b, Local and nonlocal resistances measured in a t-BLG device (D1) with a 1.68° twist angle at 80 K. The three resistance maxima of local resistance correspond to the Dirac points (at charge neutrality) and the superlattice bandgaps (at \( n = \pm n_s \approx \pm 6.50 \times 10^{12} \text{ cm}^{-2} \)). Pronounced nonlocal responses are observed inside the superlattice bandgaps. Inset: Optical image of a t-BLG device (D1). Scale bar: 4 \( \mu \text{m} \). c, The calculated moiré band structure of 1.68° t-BLG. Two moiré Dirac bands appear in the red shaded region. d, Schematic torus illustrating the first moiré Brillouin zone. Two wannier centers of the two moiré Dirac bands along circle 1 are computed, and their counterflow along circle 2 is depicted in e. e, Two red traces illustrating the nontrivial wannier-center counterflow winding, and the crossings labeled by 0 and \( \pi \) are symmetry-enforced stable points. f, Illustration of the counter-propagating edge states per spin-valley (dashed curves) in the superlattice bandgaps. The edge states acquire gaps (solid curves) due to symmetry breaking at t-BLG boundaries.

Figure 2 | Displacement field dependence of local and nonlocal resistances. a, Local resistance map as a function of \( V_{BG} \) and \( V_{TG} \). Inset: Optical image of dual-gate device (D2) with a scale bar of 4 \( \mu \text{m} \). b, Nonlocal resistance measured as a function of \( V_{BG} \) and \( V_{TG} \). The gray dashed lines denote several different displacement fields. Pronounced nonlocal responses are observed at around the two superlattice bandgaps at \( n = \pm n_s \). All data were taken from D2 at 80 K.

Figure 3 | Twist angle dependence of nonlocal resistance and DOS. Measured nonlocal resistance (red curves) and calculated density of states (DOS) as functions of \( n \) measured in various t-BLG devices (D3 to D7) with different twist angles from \( \sim 1.3^\circ \) to \( \sim 1.9^\circ \) at 80 K. (See Extended Table 1 for device details.) Nonlocal resistance peaks appear at the DOS minima corresponding to the superlattice bandgaps in each t-BLG.

Figure 4 | Length and temperature dependence of nonlocal resistance. a, Length dependence of nonlocal responses in a multiterminal device (D8) measured at 80 K. Three sets of \( R_{NL} \) are measured by driving current \( I \) and probing voltage drop \( V \) using different pairs of terminals as indicated in the figure legend. Top left inset: Optical image of D8. Scale bar: 3 \( \mu \text{m} \). Middle inset:
Semi-log plot of $R_{NL}$ peaks versus channel length $L$. The nonlocal responses exponentially decay with $L$. Solid points and circles represent the electron- and hole-side $R_{NL}$ peak values, respectively. The fittings (dashed lines) yield diffusion lengths of 1.2 and 1.4 μm for electron and hole sides, respectively. b, Scaling relation between $R_{NL}$ and $R_L$ measured in D9 at different temperatures. Data points around the $R_{NL}(R_L)$ peaks are extracted in the range $n \pm \Delta n = 5.54 \pm 0.22$ and $-5.54 \pm 0.28$ (10^{12} \text{cm}^{-2}) for the electron (orange shaded region) and hole (green shaded region) sides. A linear relation between $\ln R_{NL}$ and $\ln R_L$ gives a slope 3.00 (2.51), 3.37 (2.36), 3.01 (2.17) and 3.50 (2.29) for hole-side (electron-side) responses at 80, 90, 100, and 110 K, respectively. c, Temperature dependence of $R_{NL}$ from 80 K up to room temperature. Inset: Semi-log plot of $R_{NL}$ peak values versus $100/T$. Above 80 K, $R_{NL}$ also exhibits thermal activation behavior with the activation energies extracted to be $157 \pm 20 \text{meV}$ and $129 \pm 16 \text{meV}$ for the electron and hole sides, respectively.

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Figure 1: Signature of band topology in small-twist-angle bilayer graphene
Figure 2: Displacement field dependence of local and nonlocal resistances

Figure 3: Twist angle dependence of nonlocal resistance and DOS
Figure 4: Length and temperature dependence of nonlocal properties

(a) Length dependence of nonlocal properties.

(b) Log-log plot of nonlocal resistance versus temperature for different voltages.

(c) Temperature dependence of nonlocal resistance peak for different temperatures.