Identification of superconducting pairing symmetry in twisted bilayer graphene using in-plane magnetic field and strain

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We show how the pairing symmetry of superconducting states in twisted bilayer graphene can be experimentally identified by theoretically studying effects of externally applied in-plane magnetic field and strain. In the low field regime, superconducting critical temperature $T_c$ is suppressed by in-plane magnetic field $B_{\parallel}$ in singlet channels, but is enhanced by weak $B_{\parallel}$ in triplet channels, providing an important distinction. The in-plane angular dependence of the critical $B_{\parallel,c}$ has a six-fold rotational symmetry, which is broken when strain is present. We show that anisotropy in $B_{\parallel,c}$ generated by strain can be similar for $s$- and $d$-wave channels in moiré superlattices. The $d$-wave state is pinned to be nematic by strain and consequently gapless, which is distinguishable from the fully gapped $s$-wave state by scanning tunneling measurements.

Introduction. — The groundbreaking discovery\textsuperscript{1,2} of correlated insulating and superconducting (SC) states in twisted bilayer graphene (TBG) has opened the door to study many-body physics using versatile moiré bilayers. These initial findings have been verified and expanded\textsuperscript{3,4} spanning almost the full gamut of solid-state physics. All these SC channels have been theoretically stimulated a large number of theoretical studies\textsuperscript{12–47} and anomalous Hall effect at certain filling factors\textsuperscript{6,10}. These remarkable discoveries have stimulated a large number of theoretical studies\textsuperscript{12–47} spanning almost the full gamut of solid-state physics from single-particle band structure theory to many-body theory. A key question in this context is the nature of the superconducting pairing symmetry, particularly whether any non-$s$-wave exotic pairing plays a role in TBG.

In this Letter, we focus on TBG SC states, which can be classified into $s$, $p$, $d$ and $f$ pairing channels based on the $D_6$ point group symmetry and spin SU(2) symmetry. All these SC channels have been theoretically proposed for TBG in the current literature. The conventional $s$-wave pairing can arise from the enhanced electron-phonon interaction in the TBG flat bands\textsuperscript{43–47}. The unconventional pairing with $p$, $d$ or $f$ wave symmetry can be induced by electron-electron Coulomb repulsion\textsuperscript{21,24}, but can also be mediated by electron-phonon interaction\textsuperscript{43,44} due to TBG band symmetries, e.g., sublattice pseudospin chirality and valley symmetry.

An important question is how the pairing symmetry in the TBG SC states can be experimentally identified. We address this question by theoretically studying the response of SC states in each pairing channel to in-plane magnetic field $B_{\parallel}$ and strain. We show that the dependence of SC critical temperature $T_c$ on $B_{\parallel}$ in the low field regime distinguishes spin singlet ($s,d$) from triplet ($p,f$) pairings. In particular, $T_c$ is suppressed by $B_{\parallel}$ in singlet channels, but is enhanced by weak $B_{\parallel}$ in triplet channels. When compared to the first experiment\textsuperscript{4}, our theory indicates that the TBG SC states has spin singlet pairing. For the singlet channels, $s$-wave state is fully gapped, while the $d$-wave state in the presence of strain is nematic and gapless. Therefore, $s$- and $d$-wave states can be distinguished by scanning tunneling gap measurement in the presence of weak strain.

Moiré Hamiltonian. — The single-particle TBG physics with small twist angle $\theta$ is described by the continuum moiré Hamiltonian\textsuperscript{48}, which is independent of spin and is given in valley $\tau K$

$$\mathcal{H}_\tau = \begin{pmatrix} T_{\tau}(r) & h_{\tau \ell}(k) \\ T_{\tau}^\dagger(r) & h_{\tau \ell}(k) \end{pmatrix},$$

where $h_{\tau \ell}$ is the Dirac Hamiltonian for layer $\ell$, and $T_{\tau}$ is the interlayer tunneling that varies spatially with the moiré period. Both $h_{\tau \ell}$ and $T_{\tau}$ can be specified using Pauli matrices $\sigma_x, \sigma_y, \sigma_z$ in the sublattice space as follows

$$h_{\tau \ell}(k) = \hbar v_F e^{-i\tau \ell \delta x} [\mathbf{k} - \tau (\kappa_\ell) \cdot (\tau \sigma_x, \sigma_y)] e^{i\tau \ell \gamma z},$$

$$T_{\tau}(r) = T_{\tau}^{(0)} + e^{-i\tau \ell b \cdot r} T_{\tau}^{(+)} + e^{-i\tau \ell b \cdot r} T_{\tau}^{(-)} = w_0 \sigma_0 + w_1 \left( \cos \frac{2j\pi}{3} \sigma_x + \tau \sin \frac{2j\pi}{3} \sigma_y \right),$$

where $\tau = \pm$ is the valley index, $\ell$ is $+1$ and $-1$, respectively, for bottom (b) and top (t) layers. $b_\ell$ are moiré reciprocal lattice vectors given by $[4\pi/(\sqrt{3}a_M)](\pm 1/2, \sqrt{3}/2)$, and momentum $\kappa_\ell$ is equal to $[4\pi/(3a_M)](-\sqrt{3}/2, -\ell/2)$ which connects the center ($\gamma$) and one corner of the moiré Brillouin zone. $a_M$ is the moiré period approximated by $a_0/\theta$, where $a_0$ is the monolayer graphene lattice constant. We use the same parameter values for $(v_F, w_0, w_1)$ as in Ref.\textsuperscript{44}.

We now discuss how the moiré Hamiltonian in Eq.\textsuperscript{4} is modified by an in-plane magnetic field $B_{\parallel}$ and a strain field. The field $B_{\parallel}$ generates a layer-dependent gauge field $A_{\parallel} = -\ell d_z (B_{\parallel} \times \hat{z})/2$, where $d_z$ is the interlayer distance. The momentum $k$ in $h_{\tau \ell}$ is then replaced by $k + e_0 A_{\parallel}/\hbar$, where $e_0$ is the elementary charge. Besides this orbital effect, the magnetic field also leads to the
Zeeman splitting term $\mu_B B \cdot s \cdot B_{\parallel}$, where $\mu_B$ is the Bohr magneton and $s$ are spin Pauli matrices.

To study strain effect, we consider principal strains $\epsilon_1$ and $\epsilon_2$ respectively along two orthogonal directions $n_1 = (\cos \phi, \sin \phi)$ and $n_2 = (-\sin \phi, \cos \phi)$ such that a vector parallel to $n_i$ is rescaled by a factor of $1 + \epsilon_i$. This strain then transforms a generic vector $\mathbf{R}$ to $(\hat{I}_0 + \hat{E}) \mathbf{R}$, where $\hat{I}_0$ is identity matrix and $\hat{E}$ is strain tensor defined as $\epsilon_1 n_1 \otimes n_1 + \epsilon_2 n_2 \otimes n_2$.

We consider homostRAIN with the same strain field applied to bottom and top graphene layers (Heterostrain can be studied similarly). Strain modifies the Dirac Hamiltonian $h_{\mathbf{r} \ell}$ by shifting the Dirac point [50] as captured by the following Hamiltonian,

$$h_{\mathbf{r} \ell}^{(1)} = (\epsilon_1 - \epsilon_2) - \frac{\hbar v_F}{2} \partial_{\mathbf{a}_{CC}} \ln |t_0| \begin{pmatrix} 0 & e^{i \tau (2 \phi + i \theta)} \\ e^{-i \tau (2 \phi + i \theta)} & 0 \end{pmatrix},$$

where $t_0$ and $a_{CC}$ are respectively the nearest-neighbor hopping parameter and distance in monolayer graphene. Another effect of strain is that the momentum space vector $\kappa_r$ is transformed to $(\hat{I}_0 + \hat{E})^{-1} \kappa_r$, and the same transformation also applies to $\hat{b}_s$.

We assume that SC states in TBG have one of the pairing symmetries ($s$, $p$, $d$, $f$), and study effects of $B_{\parallel}$ and $\hat{E}$ fields on each channel in the following.

$s$-wave pairing. — The $s$-wave channel can be realized by intrasublattice spin-singlet pairing. An $s$-wave pairing Hamiltonian can be derived from local on-site attractive interactions $[43]$, and is given by

$$H_0 = -g_0 \sum_{\tau_i, \sigma, \ell} \int d\mathbf{r} \psi_{\tau_i, \sigma \ell}^\dagger \hat{\psi}_{\tau_i, \sigma \ell} + \psi_{\tau_i, \sigma \ell}^\dagger \hat{\psi}_{\tau_i, \sigma \ell} + \psi_{\tau_i, \sigma \ell}^\dagger \hat{\psi}_{\tau_i, \sigma \ell},$$

where $\tau_i$ are valley indices with the constraint $\tau_1 + \tau_2 = \tau_3 + \tau_4$, and $\sigma$ represents sublattices $A$ and $B$. We use $\uparrow$ (↓) to represent spin parallel (antiparallel) to $B_{\parallel}$. The $s$-wave pair amplitudes for intervalley, intrasublattice and opposite-spin pairing are

$$\Delta_{s,\ell}(r) = s \langle \hat{\psi}_{\tau \ell \sigma(-\sigma)}(r) \hat{\psi}_{\tau \sigma \ell} \rangle = \sum_b e^{ib \cdot r} \Delta_{s,\ell, b},$$

where $\sigma$ and $s$ in the subscript represent opposite spins, $s$ in the prefactor is $+1(-1)$ for spin $\uparrow(\downarrow)$, and $b$ represents moiré reciprocal lattice vectors. We make the ansatz that the pair amplitudes $\Delta_{s,\ell}(r)$ have the moiré periodicity and therefore, can be parametrized using harmonic expansion. The linearized gap equation is then given by

$$\Delta_{s,\ell, b} = \sum_{b', \ell'} \chi_{b', \ell'}^{b, \ell}(s) \Delta_{\ell', \ell} + \Delta_{\ell, \ell', b'},$$

where the overlap function $O_{b, \ell}$ and the kernel function $K_{s, s'}$ are respectively defined as

$$O_{b, \ell} = \langle u_{n_1}(q, B_{\parallel}) | u_{n_2}(q, -B_{\parallel}) \rangle \delta_{b, \ell'},$$

$$K_{s, s'} = \frac{1 - n_F (\varepsilon_n(q, B_{\parallel}) + s \varepsilon_Z) - n_F (\varepsilon_n(q, -B_{\parallel}) + s' \varepsilon_Z)}{\varepsilon_n(q, B_{\parallel}) + s \varepsilon_Z + \varepsilon_n(q, -B_{\parallel}) + s' \varepsilon_Z - 2 \mu}. \tag{8}$$

In Eq. (8), $\mu$ is the chemical potential and $n_F$ the Fermi-Dirac occupation function. $u_{n_1}(q, \pm B_{\parallel})$ is the wave function of the $n$th moiré band at momentum $q$ in valley $+K$ for one spin component and in the presence of in-plane magnetic field $\pm B_{\parallel}$: $\varepsilon_n(q, \pm B_{\parallel})$ is the corresponding energy without including the Zeeman energy, while the Zeeman energy is taken into account by $\varepsilon_Z = \mu_B |B_{\parallel}|$.

The overlap function $\langle \cdots \rangle_{b, \ell}$ represents the layer-resolved matrix element of the plane-wave operator $e^{i b \cdot r}$. The SC critical temperature $T_c$ and critical $B_{\parallel}$ are obtained by solving Eq. (7).

Spin $\uparrow$ and $\downarrow$ bands are shifted by opposite energies due to the Zeeman effect, which leads to pair breaking for opposite spin pairing as in the $s$-wave channel [Fig. 1(a)]. The orbital effect of $B_{\parallel}$ also results in depairing, because $\varepsilon_n(q, B_{\parallel}) \neq \varepsilon_n(q, -B_{\parallel})$.

$d$-wave pairing. — The $d$-wave channel can be realized by intersublattice spin-singlet pairing, which can be mediated by intervalley optical phonons [43] as described by the following pairing Hamiltonian

$$H_d = -g_d \sum_{s, s', \ell, \sigma \neq \sigma'} \int d\mathbf{r} \hat{\psi}_{\sigma \ell}^\dagger \hat{\psi}_{-\sigma' \ell} \hat{\psi}_{\sigma' \ell} \hat{\psi}_{\sigma \ell'}.$$
where the main difference with Eq. (5) is in the sublattice dependence. The d-wave pair amplitudes are given by

\[ \Delta^{(+)}_{s,f}(r) = s(\hat{\psi}_{-Bt(-s)}(r)\hat{\psi}_{+Ats}(r)) = \sum_b e^{ib\cdot r}\Delta^{(+)}_{s,f,b}, \]

\[ \Delta^{(-)}_{s,f}(r) = s(\hat{\psi}_{-At(-s)}(r)\hat{\psi}_{+Bts}(r)) = \sum_b e^{ib\cdot r}\Delta^{(-)}_{s,f,b}, \]

(10)

where \( \Delta^{(+)}_{s,f,b} \) and \( \Delta^{(-)}_{s,f,b} \) are defined as in Eq. (5). The kernel function \( K_{s,(-s)} \) is the same as in the s-wave case, and the Zeeman effect also leads to depairing for d-wave. However, the overlap functions \( \Omega_{b,f,L} \) are different for the two channels, because of their different sublattice dependences.

When the D6 symmetry is preserved (i.e., magnetic field \( B_y \) and strain are absent), the d-wave linearized gap equation leads to two degenerate states that can be classified as \( d_x^2 - y^2 \) and \( d_y \) nematic states (alternatively, \( d + id \) and \( d - id \) chiral states). The two-component nature of the d-wave pairing is characterized by a nematic director that can be chosen as

\[ \eta \equiv (\eta_x, \eta_y) = \left( \frac{\Delta_{s,↑}^{(+)} - \Delta_{s,↓}^{(-)}}{\sqrt{2}}, \frac{\Delta_{s,↑}^{(-)} + \Delta_{s,↓}^{(+)}}{\sqrt{2}} \right) \big|_{r=0}, \]

(12)

where \( \eta \) is the angle in the moiré pattern. The \( d_x^2 - y^2 \) and \( d_y \) states respectively correspond to \( \eta \propto (1,0) \) and \( \eta \propto (0,1) \), and their degeneracy at \( T_c \) is lifted by magnetic and strain fields. A nematic order parameter can be further defined as

\[ N = (|\eta_x|^2 - |\eta_y|^2, 2\eta_x\eta_y + \eta_y^2\eta_x), \]

(13)

which is gauge invariant and will be used to characterize the d-wave states in the following.

**f-wave pairing.**—The f-wave channel can be realized by intrasublattice spin-triplet pairing, which can be mediated by acoustic phonons \( [44] \). An in-plane magnetic field \( B_x \) favors equal spin pairings in the f-wave channel. The equal-spin f-wave pairing Hamiltonian is given by

\[ H_f = -g_f \sum_{\sigma,\ell} \sum_{s=\uparrow,\downarrow} \int d\mathbf{r} \hat{\psi}_{+\sigma ts}^\dagger \hat{\psi}_{-\sigma ts}^\dagger \hat{\psi}_{-\sigma ts} \hat{\psi}_{+\sigma ts}. \]

(14)

The analysis of p-wave channel is similar to the d-wave except for the difference of equal spin pairing. The Zeeman effect plays the same role in p- and f-wave channels.

**Critical \( B_{||} \).**—We calculate the in-plane critical magnetic field as a function of temperature. Representative results in the absence of strain field are plotted in
The two effective chemical potentials (DOS) is, respectively, enhanced and suppressed at the two spin components. Quite generally, the density of states is suppressed slightly by the weak Zeeman effect, which leads to different effective chemical potentials.

The Zeeman effect reach 1.

Uniaxial strain pins the nematic order parameter $\hat{C}_3$ to a particular direction. For example, tensile strain applied along $\hat{x}$ ($\hat{y}$) favors $d_{xy}$ ($d_{x^2-y^2}$) nematic state, similar to the effect of in-plane magnetic field.

In the presence of a fixed uniaxial strain, the angular variation of the in-plane critical magnetic field $B_{\parallel,c}$ is twofold (instead of sixfold) rotational symmetric. The strain can lead to similar anisotropy in $B_{\parallel,c}$ for $s$- and $d$-wave channels [Figs. 2(c) and 2(d)], because the nearly flat moiré bands near magic angle are sensitive to tiny strain. This raises the question how $s$- and $d$-wave channels can be distinguished experimentally. We propose that scanning tunneling microscopy (STM) study of the SC gap can be used for the distinction. In particular, the $s$-wave superconductivity is fully gapped [Fig. 3(a)]. In contrast, the nematic $d$-wave state, which is pinned by strain, is gapless with point nodes [Fig. 3(b)].

**Discussion.** — Strain has been found to be generally presented in TBG devices from STM imaging. Recent transport study shows that in-plane critical transport study shows that in-plane critical transport study [54] shows that in-plane critical transport study [54] shows that in-plane critical transport study [54] shows that in-plane critical transport study [54].
This two-fold anisotropy in $B_{\parallel,c}$ might be a signature of nematic state, because SC states with a two-component order parameter such as $d$-wave channel have been argued to be more susceptible to strain compared to $s$-wave states in bulk materials [52, 55]. However, we note that moiré band structure itself can be very sensitive to strain due to the narrow bandwidth, and our calculation indicates that strain can in principle lead to similar anisotropy in $B_{\parallel,c}$ for $s$- and $d$-wave channels. Therefore, we suggest that a tunneling measurement of SC gap could provide a more conclusive distinction between these two pairing states.

Evidences of superconductivity have recently been reported also in other moiré systems, for example, ABC trilayer graphene on boron nitride [50] and twisted double bilayer graphene [57–59]. Our theory can be generalized to these related systems. In twisted double bilayer graphene, in-plane magnetic field has been found to enhance $T_c$ in the low field regime [55], which has been interpreted as an indication of spin triplet pairing [58 [50]; our theory supports this interpretation.

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Strain preserves \( T \) symmetry and \( C_{2z} \) symmetry, but breaks other rotational symmetries around \( \hat{z} \) axis. Again, \( C_{2z} T \) symmetry is preserved and Dirac cones remain gapless with movable Dirac touching points. When \( B_\parallel \) or strain is along one of the in-plane twofold rotation axes, there is a two-fold rotational symmetry around this axis.

We denote the moiré band energy (without including Zeeman term) as \( \varepsilon_{n,T}(q, B_\parallel) \), where \( n \) is the band index and \( T \) is the valley index. Because time reversal operation flips \( \tau \) and \( B_\parallel \), we have the identity \( \varepsilon_{n,T}(q, B_\parallel) = \varepsilon_{n,-T}(-q, -B_\parallel) \), which has been used to simplify the pair susceptibilities, for example, Eq. (8) of the main text.

**ORBITAL EFFECT OF MAGNETIC FIELD ON \( T_e \)**

We show that the leading orbital effect of in-plane magnetic field on \( T_e \) is second order, while the Zeeman splitting has a dominant first order effect on \( T_e \) for the spin triplet channel in the low field regime.

For definiteness, we consider in-plane magnetic field \( B_\parallel \) along \( \hat{x} \) direction with \( B_\parallel = B \hat{x} \). We use \( \rightarrow \) and \( \leftarrow \) to indicate spin pointing to \( +\hat{x} \) and \( -\hat{x} \) directions, respectively. The Zeeman splitting is denoted as \( \varepsilon_x = \mu_B B \), where \( \varepsilon_x \) can be positive or negative depending on \( B \). For equal spin pairing, \( \rightarrow \) and \( \leftarrow \) spin components have independent linearized gap equations. To demonstrate the effect of \( B_\parallel \), we consider \( \rightarrow \) spin component in the \( f \)-wave channel, of which the pair susceptibility is

\[
\chi_{\rightarrow}(B_\parallel, \varepsilon_x) = \frac{g_f}{4 \Lambda} \sum_{q} K_{\rightarrow} |O|^2, \quad O = \langle u(q, B_\parallel) | u(q, -B_\parallel) \rangle, \quad K_{\rightarrow} = \frac{1 - n_f \langle \varepsilon(q, B_\parallel) + \varepsilon_x \rangle - n_f \langle \varepsilon(q, -B_\parallel) + \varepsilon_x \rangle}{\varepsilon(q, B_\parallel) + \varepsilon(q, -B_\parallel) - 2(\mu - \varepsilon_x)},
\]

where we have retained only the moiré band that crosses the Fermi energy, and the \( b = 0 \) component of the susceptibility. The bottom and top graphene layers are assumed to have the same pair amplitudes in Eq. (17). These simplifications make the analysis more straightforward.

Equation (17) shows that \( \chi_{\rightarrow}(B_\parallel, \varepsilon_x) = \chi_{\rightarrow}(-B_\parallel, \varepsilon_x) \), i.e. \( \chi \) remains the same when the magnetic field changes sign only in the orbital effect but not in the Zeeman effect. Therefore, the orbital effect of magnetic field on \( T_e \) is at least second order. The Zeeman splitting effectively shifts the chemical potential \( \mu \) to \( \mu - \varepsilon_x \), which results in a first-order correction to \( T_e \) as given by

\[
k_B T_{\rightarrow, c} \approx \Lambda \exp\left\{ -\frac{1}{g_f D(\mu - \varepsilon_x)} \right\} = \Lambda \exp\left\{ -\frac{1}{g_f D(\mu)} \right\} \left[ 1 - \frac{D'(\mu)}{g_f D(\mu)} \right] B, \quad (18)
\]

where \( \Lambda \) is an energy cutoff, \( g_f = g_f / 4 \), and \( D(\mu) \) is the DOS. The variation of DOS with \( \mu \) leads to a linear \( B \) correction to \( T_e \) in the triplet channel.

It can be shown in a similar way that both orbital and Zeeman effects lead to second-order corrections to \( T_e \) for spin singlet channels.
GINZBURG-LANDAU THEORY FOR $d$-WAVE CHANNEL

The $d$-wave state has a two-component pairing order parameter. As demonstrated in the main text, the nematic director $\eta$ can be steered by in-plane magnetic field and strain field, which is captured by the phenomenological Ginzburg-Landau free energy

$$
\mathcal{F}_d = \alpha [T - (T_c(0) - \beta |B_\parallel|^2)](|\eta_x|^2 + |\eta_y|^2) \\
+ |\lambda_1 (B_x^2 - B_y^2) + \lambda_2 (\mathcal{E}_{xx} - \mathcal{E}_{yy})||\eta_x|^2 - |\eta_y|^2) \\
+ (2 \lambda_1 B_x B_y + 2 \lambda_2 \mathcal{E}_{xy})(\eta_x^* \eta_y + \eta_y^* \eta_x),
$$

where we keep leading order terms, in particular, second order terms in $\eta$ and $B_\parallel$, and first order terms in strain. $\mathcal{E}_{xx}$ and $\mathcal{E}_{yy}$ are diagonal terms in the symmetric strain tensor $\mathcal{E}$, and $\mathcal{E}_{xy}$ is the off-diagonal term. The numerical results shown in Figs. 2 and 3 of the main text correspond to $\lambda_1 > 0$ and $\lambda_2 > 0$ such that $d_{xy}$ ($d_{x^2-y^2}$) state is preferred when $B_\parallel$ or tensile strain is along $\hat{x}$ ($\hat{y}$). Because the free energy $\mathcal{F}_d$ in Eq. (19) only includes terms up to second order, it does not fully capture the angular variation of the in-plane critical magnetic field $B_{\parallel,c}$ shown in Fig. 2(b) of the main text.