Effect of Defects in Superconducting Phase of Twisted Bilayer Graphene

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(Dated: August 29, 2019)

In this work we study the effect of impurity in the superconducting phases of the twisted bilayer graphene (TBG) by analysing bound states induced by the impurity. As a comparison with the superconducting phase, we first consider the impurity effect in the TBG without superconductivity in the scheme of a low energy effective theory. For superconductivity, our basis is a four-band model with different superconducting pairing symmetries. Then we construct the effective impurity Hamiltonian and compute the local density of state (DOS). We find that for different kind of pairing symmetries the numbers of bound states are different. These results can in principle be detected in scanning tunnelling microscopy (STM) experiments, and therefore the pairing symmetry may be determined. Finally we consider the multi-impurity effect and compute phase diagrams in terms of effective gap and the strength and density of impurities. We find that in \((p + ip)\)-wave and \((d + id)\)-wave phases superconductivity will be destroyed by impurities with strong strength or concentration.

I. INTRODUCTION

Twisted bilayer graphene (TBG) has attracted much interest these days. The most striking property of TBG is that flat bands emerge at the magic angle \(\theta = 1.08^\circ\). Recently it has been found that flat bands will result in rich physics. An insulating phase was discovered at the filling of \(n = 2\). This insulating phase was argued to be a Mott insulator. Around the insulator phase, superconducting phases were observed by doping slightly away from the insulator phase. Different theories giving rise to different pairing symmetries have been proposed to explain the superconducting phases. However, the pairing symmetry of the order parameter in superconducting phase of the TBG system is still under debate. One experimental method to identify the pairing symmetry in TBG has been proposed in Ref. which subjects the TBG to an external magnetic field and strain. In this work we propose another method to distinguish the pairing symmetry in TBG by studying the impurity induced bound states in the superconductor phases.

Impurities in superconductor may give rise to different phenomena for different pairing mechanism and different pairing symmetry. A nonmagnetic impurity will not break the Cooper pair in an \(s\)-wave superconductor, but it can break Cooper pairs with \(p\)-wave and \(d\)-wave symmetry and may induce bound states or quasi-bound states inside the superconducting gap. A magnetic impurity may induce Kondo effect in the superconducting phase. In multi-impurity case, when the strength and density of impurities is large, the superconducting phase coherence will be destroyed, which converts the system to a normal phase. Since disorder such as carbon vacancy and adatom is unavoidable in graphene, it is necessary to study the effect of impurities in TBG.

We study the effect of impurity by calculating the number of impurity induced in-gap states for different pairing symmetry, from which we can get some knowledge about the pairing symmetry in the TBG system. However, we do not consider the correlation between electrons, which is also believed to be important in TBG. The in-gap states can be observed in STM experiments and may serve as an experimental indicator of the pairing symmetries. This paper is organized as follows. In Sec II, we consider the impurity effect in the normal phase of TBG. We find that the local density of state (DOS) in the two bands next to the nearly flat bands proposed by Ref. is suppressed by the impurity. In Sec III, we consider the impurity effects in superconducting phases. We consider both single impurity effect and multi-impurity effect and calculate the DOS. We find that in the single impurity case the number of bound state is different for different pairing symmetries. In the multi-impurity case we calculate the effective superconducting gap as a function of the effective strength of impurities which shows the extinction of superconductivity in \((d + id)\)-wave phase and...
We give a conclusion in Sec IV and the calculation details are listed in Appendix.

II. DISORDER EFFECT IN THE NORMAL PHASE OF TBG

In this section we consider a single impurity located in the twisted bilayer graphene. We use Moiré bands Hamiltonian\(^{11}\) to describe the system without impurities. Constraining the momentum close to the Dirac point, we have the Moiré bands Hamiltonian\(^{11}\)

\[
H_{\vec{k}\vec{k}'} = \delta_{\vec{k}\vec{k}'} \begin{pmatrix}
  h_{\vec{k}}(\frac{\theta}{2}) & wT_1 & wT_2 & wT_3 \\
  wT_1 & h_{\vec{k}}(-\frac{\theta}{2}) & 0 & 0 \\
  wT_2 & 0 & h_{\vec{k}}(-\frac{\theta}{2}) & 0 \\
  wT_3 & 0 & 0 & h_{\vec{k}}(-\frac{\theta}{2})
\end{pmatrix}
\]

where \(w = 110\) meV is the strength of hopping, \(\vec{k}_j = \vec{k} + \vec{q}_j\) and \(\vec{q}_j\) are defined in FIG. 2. The matrix elements (which are all two by two matrices) of the Hamiltonian above are defined as\(^{11}\)

\[
h_{\vec{k}}(\theta) = -v \kappa \begin{pmatrix}
  0 & e^{-i\theta_{\vec{k}-\theta}} \\
  e^{i\theta_{\vec{k}-\theta}} & 0
\end{pmatrix},
\]

\[
T_1 = \begin{pmatrix}
  1 & 1 \\
  1 & 1
\end{pmatrix},
\]

\[
T_2 = \begin{pmatrix}
  e^{-i\frac{\pi}{4}} & 1 \\
  e^{i\frac{\pi}{4}} & e^{-i\frac{\pi}{4}}
\end{pmatrix},
\]

\[
T_3 = \begin{pmatrix}
  e^{i\frac{\pi}{4}} & 1 \\
  e^{-i\frac{\pi}{4}} & e^{i\frac{\pi}{4}}
\end{pmatrix},
\]

where \(h_{\vec{k}}(\theta)\) is the Hamiltonian of graphene and \(v\) is the Dirac velocity. Besides, \(\vec{k}\) is measured from Dirac point. Dispersion relations around Dirac point is shown in FIG. 3.

![FIG. 2. The three \(q_j\) defined in Moiré Brillouin zone and directions of \(k_x\) and \(k_y\).](image)

We consider the impurity potential in real space as \(U_{imp}(\vec{r}) = u_0 \delta(\vec{r} - \vec{R}_0^{A(A')})\), where \(u_0\) is the strength of the potential and \(\vec{R}_0^{A(A')}\) is the location of the impurity on \(A (B)\) site. The impurity Hamiltonian is

\[
\tilde{H}_{\text{imp}} = \int d\tilde{r} c^\dagger_{+,A,\vec{r}}U_{\text{imp}}(\tilde{r})c_{+,A,\vec{r}},
\]

where \(c^\dagger_{+,(-),\vec{R}_0^{A(A')}}\) is the creation (annihilation) operator on \(A (B)\) site of the top (bottom) layer. We consider that the impurities only affect one layer of the TBG. Without losing generality, we locate the impurity on site \(A\) on the upper layer.

In the basis of Hamiltonian defined in Eq. (1), the impurity Hamiltonian reads

\[
(H_{\text{imp}})_{\vec{k}\vec{k}'} = u_0\epsilon^{i(\vec{k}'-\vec{k})}R_0^{A(A')}\begin{pmatrix}
  I_{2\times 2} & 0 & 0 & 0 \\
  0 & 0 & 0 & 0 \\
  0 & 0 & 0 & 0 \\
  0 & 0 & 0 & 0
\end{pmatrix},
\]

where \(I_{2\times 2}\) is a two by two identity matrix.

We compute the local DOS by a standard method\(^{13}\) The local DOS is showed in FIG. 4. From these figures we find that the impurity will suppress the local DOS of the two bands near to the flat bands (as shown in FIG. 3) at the location of impurity. From FIG. 4(b)-4(g), we can also conclude that for impurity in AA, AB or BA region, there is no significant difference in the local DOS.

III. BOUND STATE INDUCED BY IMPURITIES IN SUPERCONDUCTING PHASE OF TBG

A. Model and Pairing Symmetry

The Hamiltonian proposed by Ref.\(^{11}\) can only describe the physics when \(\vec{k}\) is close to the Dirac points. However, the superconductivity likely involves the property of bands in the whole Brillouin zone. Therefore, we have

![FIG. 3. Dispersion relations of Bistritzer-MacDonald model around Dirac point. One feature of this model is that at \(\epsilon_k\) around \(\pm 1\) meV there are two nearly flat bands.](image)
to find an alternative theory as the platform. Some previous works have proposed different models for the TBG. Among these models, we choose the four-band tight-binding model proposed by Ref[2]. In this model, the basis in real space is \( \{p_x, p_y, p_x', p_y'\} \), where \( x \) and \( y \) denote \( p_x \) and \( p_y \) orbits, as well as \( A \) and \( B \) denote different kinds of sites. The Hamiltonian in \( k \)-space reads[20]

\[
H(\vec{k}) = \begin{pmatrix} h_{11} & h_{12} & h_{13} & h_{14} \\ h_{21}^* & h_{22} & h_{23} & h_{24} \\ h_{31}^* & h_{32} & h_{33} & h_{34} \\ h_{41}^* & h_{42} & h_{43} & h_{44} \end{pmatrix},
\]

where each component is a function of \( \vec{k} = (k_x, k_y) \) given by Supplementary Materials of Ref[20]. To describe the superconductivity, we introduce the 8-component Nambu spinor

\[
\Psi_{\vec{k}} = \begin{pmatrix} \Phi_{\vec{k}} \\ \Phi_{\vec{k}}^\dagger \end{pmatrix},
\]

where \( \Phi_{\vec{k}} \) is the basis in which the Hamiltonian in Eq.(8) is diagonal. For \( s \)-wave and \( d \)-wave superconductor, \( \sigma = \uparrow \) and \( \sigma' = \downarrow \), while for \( p \)-wave superconductor, \( \sigma = \sigma' = \uparrow \).

Hence, the BdG Hamiltonian has the form

\[
H_{BdG}^{\vec{k}} = \begin{pmatrix} E_{\vec{k}} & -\Delta_{\vec{k}} \\ -\Delta_{\vec{k}}^\dagger & -E_{\vec{k}} \end{pmatrix},
\]

where diagonal matrix \( E_{\vec{k}} = \text{diag}\{\epsilon_{1,\vec{k}}, \epsilon_{2,\vec{k}}, \epsilon_{3,\vec{k}}, \epsilon_{4,\vec{k}}\} \) represents the energy bands (four \( \epsilon_{k} \)'s) and \( \mu \) is the chemical potential, and \( \Delta_{\vec{k}} \) is the order parameter. Since there is no interband pairing, \( \Delta_{\vec{k}} \) is diagonal and then gains the form of \( \Delta_{\vec{k}} = S(\vec{k}) \cdot \text{diag}\{\Delta_1, \Delta_2, \Delta_3, \Delta_4\} \), where \( \Delta_4 \) is the order parameter in the \( j \)-th band and \( S(\vec{k}) \) reflects the symmetry of them. For \( s \)-wave, \( S(\vec{k}) = 1 \). For \( d \)-wave \( (d + id) \),

\[
S(\vec{k}) = \cos(\sqrt{3} k_x + \frac{1}{2} k_y) - \cos(\sqrt{3} k_x - \frac{1}{2} k_y) + i \cdot \sin(\sqrt{3} k_x + \frac{1}{2} k_y) \sin(\sqrt{3} k_x - \frac{1}{2} k_y).
\]

For \( p \)-wave \( (p + ip) \),

\[
S(\vec{k}) = \sin(\sqrt{3} k_x + \frac{1}{2} k_y) + i \cdot \sin(\sqrt{3} k_x - \frac{1}{2} k_y).
\]

The values of \( k_x \) and \( k_y \) are measured in the unit of \( 2\pi/\alpha \) where \( \alpha \) is the lattice constant defined in Ref[20], and their directions are defined in FIG. 2.
B. Construction of Impurity Hamiltonian

The model we adapted reduces the complicated TBG structure to a honeycomb lattice formed by AB and BA sites of the supercell of TBG. However, impurities can be anywhere in the TBG, not only on the AB and BA sites. For simplicity, we consider those impurities located on AA, AB and BA sites.

First, we consider a single impurity located on an AB site. The impurity potential is given by Eq.(6) in real space, with $\vec{R}_{0}^{AB}$ replaced by $\vec{R}_{0}^{AB}$ of $\vec{R}_{0}^{BA}$. Then, in Bloch representation, the Hamiltonian takes the form

$$\hat{H}_{imp}^{AB} = \sum_{\vec{k}, \vec{k}'} P^\dagger_{\vec{k}} \cdot U_{\vec{k} \vec{k}'} \cdot P_{\vec{k}'} ,$$

(11)

where

$$P_{\vec{k}} = \begin{pmatrix} p^A_{x,\vec{k}} & p^A_{y,\vec{k}} & p^B_{x,\vec{k}} & p^B_{y,\vec{k}} \end{pmatrix}^T$$

(12)

stands for annihilation operators in Bloch basis and $U_{\vec{k} \vec{k}'}$ is a four by four matrix whose elements are overlaps of Bloch wave functions and the impurity potential. Converting the expression of impurity Hamiltonian to Wannier representation, we have

$$\hat{H}_{imp}^{AB} = \sum_{\vec{k}, \vec{k}'} W^\dagger_{\vec{k}} \cdot (\hat{H}_{imp}^{AB})_{\vec{k} \vec{k}'} \cdot W_{\vec{k}'} ,$$

(13)

where $W_{\vec{k}}$ is the annihilation operators in Wannier basis and $(\hat{H}_{imp}^{AB})_{\vec{k} \vec{k}'}$ takes the form (take its (1,2)-component as an example)

$$((\hat{H}_{imp}^{AB})_{\vec{k} \vec{k}'})_{(1,2)} = u_0 \sum_{i,j} e^{-i(\vec{k} \cdot \vec{R}_{AB} - \vec{k}' \cdot \vec{R}_{AB}')} \cdot$$

$$w^A_x (\vec{R}_{0}^{AB} - \vec{R}_{AB})_{i,j} w^B_y (\vec{R}_{0}^{BA} - \vec{R}_{AB})_{i,j} ,$$

(14)

where $w^s_i (\vec{r} - \vec{R}_{AB})_{i,j} , \nu = x, y$ and $s = AB, BA$ are Wannier wave functions.

As indicated in Ref. [20], the Wannier functions are localized in AB and BA region. Therefore, the contribution of $w^s_i (\vec{R}_{0}^{AB} - \vec{R}_{AB})_{i,j} w^B_y (\vec{R}_{0}^{BA} - \vec{R}_{AB})_{i,j}$ is dominant only when $\vec{R}_{AB}^AB$ and $\vec{R}_{AB}^BA$ are close to $\vec{R}_{0}^{AB}$. The term $w^s_i (\vec{r} - \vec{R}_{AB})_{i,j} w^B_y (0)$ is about one order larger than the terms $w^s_i (\vec{r} - \vec{R}_{AB})_{i,j} w^B_y (\vec{r} - \vec{R}_{AB})_{i,j}$, while the latter two are one order larger than $w^s_i (\vec{r} - \vec{R}_{AB})_{i,j} w^B_y (\vec{r} - \vec{R}_{AB})_{i,j}$, $i, j = 1, 2, 3$. We only choose those terms above.

As a result, in Eq.(14), we only need to take account of terms that for both $i$ and $j$, $\vec{R}_{0}^{AB} - \vec{R}_{i,j}^AB$ equals to 0 or $\vec{r}_l$, $l = 1, 2, 3$. With this preparation, we can construct our Hamiltonian for impurities located on AB sites as

$$\left( H_{imp}^{AB} \right)_{\vec{k} \vec{k}'} = u \sum_{\vec{R}_{i,j}^{AB}} e^{-i(\vec{k} \cdot \vec{R}_{0}^{AB} - \vec{k}' \cdot \vec{R}_{i,j}^{AB})} \cdot$$

$$\begin{pmatrix} t_0 & 0 & 0 & 0 \\ T_{NN}^T \cdot J_{\vec{k} \vec{k}'}^* & 0 & 0 & 0 \\ 0 & 0 & t_0 & 0 \\ 0 & 0 & 0 & t_0 \end{pmatrix} ,$$

(15)

where we absorb the unit of energy into $t_0$ and $T_{NN}$, and left a dimensionless scaling factor $u$ to reflect the strength of the impurity. $\vec{R}_{i,j}^{AB}$ is the position of impurities and $J_{\vec{k} \vec{k}'} = \sum_{j=1,2,3} e^{-i(\vec{k} \cdot \vec{R}_{i,j}^{AB}) \cdot \vec{r}_j}$. The value of coefficient $t_0$ which matches $w^s_i (0) w^B_y (0)$, is about one order larger than the components of two by two matrix $T_{NN}$ which match $w^s_i (\vec{r}_j) w^B_y (0)$ and $w^s_i (0) w^B_y (\vec{r}_j)$. Besides, since the impurity Hamiltonian should conserve the point group symmetry of and time reversal symmetry, there are some restrictions on matrix $T_{NN}$. Given that the Wannier basis forms a four-dimensional representations of the point group of the TBG and the corresponding representation matrix of $C_3$ rotation is

$$C_3 = \begin{pmatrix} \cos \theta & \sin \theta & 0 & 0 \\ -\sin \theta & \cos \theta & 0 & 0 \\ 0 & 0 & \cos \theta & \sin \theta \\ 0 & 0 & -\sin \theta & \cos \theta \end{pmatrix} ,$$

(16)

where $\theta = \frac{2 \pi}{3}$. Then the impurity Hamiltonian should satisfy

$$C_3^{-1} \cdot ( H_{imp}^{AB} )_{\vec{k} \vec{k}'} \cdot C_3 = ( H_{imp}^{AB} )_{\vec{k} \vec{k}'} ,$$

(17)

which gives $T_{NN}$ the form

$$T_{NN} = \begin{pmatrix} t_{NN} & t_{NN}' \\ -t_{NN}' & t_{NN} \end{pmatrix} .$$

(18)

When superconductivity is taken accounted, the time reversal symmetry for the impurity Hamiltonian as well as the property of Hermitian requires that

$$\left( H_{imp}^{AB} \right)_{\vec{k} \vec{k}'} = \left( ( H_{imp}^{AB} )_{\vec{k} \vec{k}'} \right)^T = \left( ( H_{imp}^{AB} )_{-\vec{k} \vec{k}'} \right)^T ,$$

(19)

which further indicates that $T_{NN}$ must be a real matrix.

Swapping the two columns and two rows of $( H_{imp}^{AB} )_{\vec{k} \vec{k}'}$, we can get the Hamiltonian for impurities located on BA sites

$$\left( H_{imp}^{BA} \right)_{\vec{k} \vec{k}'} = u \sum_{\vec{R}_{i,j}^{BA}} e^{-i(\vec{k} \cdot \vec{R}_{0}^{BA} - \vec{k}' \cdot \vec{R}_{i,j}^{BA})} \cdot$$

$$\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & T_{NN}^T \cdot J_{\vec{k} \vec{k}'}^* & 0 & 0 \\ T_{NN} \cdot J_{\vec{k} \vec{k}'} & 0 & 0 & 0 \\ 0 & 0 & 0 & T_{NN} \cdot J_{\vec{k} \vec{k}'}^* \end{pmatrix} ,$$

(20)

where we have already used $( T_{imp}^{AB} )^T = T_{imp}^{BA}$.
FIG. 6. Local DOS of \((d + id)\)-wave phase with an impurity at \(AB\). (a) shows the DOS without impurity, (b) shows the local DOS at the location of the impurity which is located at \(AB\) or \(BA\) region, (c) shows the local DOS at the distance of 15 lattice constants from the location of the impurity which is located at \(AB\) or \(BA\) region, (d) shows the local DOS at the nearest \(AB\) region from the \(AA\) region where the impurity is located, (e) shows the local DOS at the nearest \(BA\) region from the \(AA\) region where the impurity is located, and (f) shows the DOS at the distance of \(32/\sqrt{3}\) lattice constants from the location of the impurity which is located at \(AA\) region, respectively. For \((d + id)\)-wave phase, there are two bound states in the gap when the impurity is located at \(AB\) or \(BA\) region and no bound state in the gap when the impurity is located at \(AA\) region.

FIG. 7. Local DOS of \((p + ip)\)-wave phase with an impurity at \(AB\). (a) shows the DOS without impurity, (b) shows the local DOS at the location of the impurity which is located at \(AB\) or \(BA\) region, (c) shows the local DOS at the distance of 10 lattice constants from the location of the impurity which is located at \(AB\) or \(BA\) region, (d) shows the local DOS at the nearest \(AB\) region from the \(AA\) region where the impurity is located, (e) shows the local DOS at the nearest \(BA\) region from the \(AA\) region where the impurity is located, and (f) shows the DOS at the distance of \(32/\sqrt{3}\) lattice constants from the location of the impurity which is located at \(AA\) region, respectively. For \((p + ip)\)-wave phase there are six bound states in the gap when the impurity is located at \(AB\) or \(BA\) region and four bound states in the gap when the impurity is located at \(AA\) region.

\[
(\mathcal{H}^A_{\text{imp}})_{k\ell} = u \sum_{\ell'} e^{-i(k - \ell') \cdot \ell^A_{\text{imp}}} \\
\left( t^{A}_{NNN} \cdot \mathbb{I}_{2 \times 2} \cdot J_{k_0} \cdot J_{0k'} \cdot t^{A}_{NNN} \cdot \mathbb{I}_{2 \times 2} \cdot J_{k_0} \cdot J_{0k'} \right)
\]

and

\[
T_{NNN} = \begin{pmatrix} t_{NNN} & t'_{NNN} \\ -t'_{NNN} & t_{NNN} \end{pmatrix},
\]

where \(t_{NNN}, t'_{NNN}, t_{NNN}, t'_{NNN}\) are real coefficients of the same order as next-nearest-neighbour hoppings whose value are around 0.1 meV\(^2\).
C. Single Impurity and Local Density of State

With preparation above, we can now calculate the local DOS by a standard method. Results are shown in FIG. 6, 7 and 8. We set $\mu = -0.165$ meV, $\Delta_1 = \Delta_2 = 0.6$ meV and $\Delta_3 = \Delta_4 = 0.8$ meV for $s$-wave phase, $\Delta_1 = \Delta_2 = \Delta_3 = \Delta_4 = 7.5$ meV for $(d + id)$-wave phase, and $\Delta_1 = \Delta_2 = 0.8$ meV and $\Delta_3 = \Delta_4 = 1.0$ meV for $(p + ip)$-wave phase. Other coefficients are set that $t_0 = 10.0$ meV, $t_{NN} = 1.5$ meV, $t'_{NN} = 1.0$ meV, $t_{NNN} = 0.2$ meV, $t'_{NNN} = 0.1$ meV, $t_{NNN} = 0.2$ meV, $t_{NNNN} = 0.1$ meV, $u = 5.0$, $\Delta_1 = \Delta_2 = 0.6$ meV and $\Delta_3 = \Delta_4 = 0.8$ meV for $s$-wave phase, $\Delta_1 = \Delta_2 = \Delta_3 = \Delta_4 = 7.5$ meV for $(d + id)$-wave phase, and $\Delta_1 = \Delta_2 = 0.8$ meV and $\Delta_3 = \Delta_4 = 1.0$ meV for $(p + ip)$-wave phase. The superconducting gaps we choose are larger than those observed in experiments; however, because of the restriction of computation resource, we have to enlarge these values to make our results numerically reliable.

The number and property of bound states varies among different superconducting phases, which gives us an effective tool to reveal the pairing symmetry in these phases. It can serve as an indicator to determine pairing symmetry of the order parameter in the superconducting phases. It can serve as an indicator to determine pairing symmetry in these phases.

D. Disorder Average and Phase Diagrams

In this section we apply disorder average to determine the multi-impurity effect and the modification induced to the DOS. Combining the BdG Hamiltonian and the

\[
\Sigma_{\vec{k}} = \Sigma_{\vec{k}}^{\underline{q}} + \Sigma_{\vec{k}-\vec{q}}^{\underline{q}} + \Sigma_{\vec{k}-2\vec{q}}^{\underline{q}}
\]

FIG. 9. Self-energy under Born approximation. Red (circle), green (box) and black nodes represent $AB$-type, $BA$-type and $AA$-type impurity scatter vertex, respectively. There is no 2-loop diagram including $AA$-type vertex. For tidiness, we omit the momenta of Green functions in 2-loop diagrams.

FIG. 10. Comparison of DOS with and without disorder average. (a) shows the DOS of $s$-wave phase without impurities, (b) shows the disorder averaged DOS of $s$-wave phase, (c) shows the DOS of $(d + id)$-wave phase without impurities, (d) shows the disorder averaged DOS of $(d + id)$-wave phase, (e) shows the DOS of $(p + ip)$-wave phase without impurities and (f) shows the disorder averaged DOS of $(p + ip)$-wave phase in which we can see that superconductivity is totally destroyed by impurities. In calculation we enlarge the value of the Lorentz broadening of Green functions to make curves more smooth.
impurity Hamiltonian, we arrive at

\[
\hat{H} = \sum_{\vec{k}, \vec{k}'} \Psi_\vec{k}^\dagger \left( H^{\text{BdG}}_{\vec{k}} \delta_{\vec{k} \vec{k}'} + \sum e^{-i(\vec{k}-\vec{k}')} \tilde{R}_{\text{imp}}^{\text{AA}} V_{\vec{k} \vec{k}'}^{\text{AB}} \right) + \sum e^{-i(\vec{k}-\vec{k}')} \tilde{R}_{\text{imp}}^{\text{BA}} V_{\vec{k} \vec{k}'}^{\text{BA}} + \sum e^{-i(\vec{k}-\vec{k}')} \tilde{R}_{\text{imp}}^{\text{BA}} V_{\vec{k} \vec{k}'}^{\text{AA}} \right) \cdot \Psi_\vec{k'},
\]

where \( \Psi_\vec{k} \) is the Nambu spinor defined in Eq. (9) and impurity scattering vertices \( V_{\vec{k} \vec{k}'}^{\text{site}} \)'s are defined as

\[
V_{\vec{k} \vec{k}'}^{\text{site}} = \begin{pmatrix} U_{\vec{k} \vec{k}'}^{\text{site}} & 0 \\ 0 & -(U_{\vec{k} \vec{k}'}^{\text{site}})^T \end{pmatrix},
\]

where \( U_{\vec{k} \vec{k}'}^{\text{site}} \) are defined in Appendix A.

On this platform, we perform disorder average to obtain the self-energy \( \Sigma_{\vec{k}} \). We only consider terms whose value are much larger or at least comparable with the next-nearest-hopping. Given that \( U_{\text{AA}}^{\text{AA}} \) is about one order smaller than other two \( U \)s, 1-loop diagram constructed by \( \text{AA} \)-type vertex has the same order as 2-loop diagrams that do not include \( \text{AA} \)-type vertex. Thus, only those Feynman diagrams showed in FIG. 9 are included in our calculation of self-energy.

The numerical result of disorder averaged DOS is shown in FIG. 10. The choice of coefficients is the same as that in Section III. C, except \( u \). Here we choose \((na^3)^2u = 0.3\), where \( n \) is the density of impurities and \( a \) is the lattice constant. We set the strength and density of the impurities on \( \text{AA} \) sites, \( \text{AB} \) sites and \( \text{BA} \) sites to be equal.

For \((d+id)\)-wave, impurities largely enhance the DOS in the gap of these phases, which is a reflection of the average effect of bound states in the gap induced by dilute impurities. For \((p+ip)\)-wave, impurities destroy the superconducting gap. For \( s \)-wave phase, since there is no bound state in the gap, the DOS is not modified much qualitatively. Besides, in numerical calculation, we find that \( \text{AA} \)-type 1-loop diagram and all the 2-loop diagrams almost have no influence on the DOS. Since the center of Wannier function is in \( \text{AB}/\text{BA} \) region, the impurity scattering effect is much weaker in \( \text{AA} \) region than that in \( \text{AB}/\text{BA} \) region. Therefore, in the dilute impurities limit, those impurities located in \( \text{AA} \) region almost do not contribute to the DOS after disorder average is applied.

Another result that can be obtained from disorder average is the phase diagram, which reflects how the effective superconducting gap relies on the density and strength of impurities, \((na^3)^2u\). Keeping other coefficients invariant, we vary \((na^3)^2u\) from 0.0 to 1.0 and find the corresponding value of the effective gap. Results are shown in FIG. 11.

According to the phase diagrams, effects of impurities in different superconductivity phases are different. In \((d+id)\)-wave phase and \((p+ip)\)-wave phase, strong or dense impurities will destroy the superconductivity while in \( s \)-wave phase they will not.

\[
\Delta_{\text{eff}} / \text{meV}
\]

FIG. 11. Phase diagrams. From this figure we can see that enough strength or concentration of impurities will destroy \((d+id)\)-wave and \((p+ip)\)-wave superconductivity, while the superconducting gap of \( s \)-wave phases can remain finite.

IV. CONCLUSION

In this work, we find that in the normal phase of TBG, an impurity in \( \text{AA} \), \( \text{AB} \) or \( \text{BA} \) region will suppress the local DOS of the two bands next to the nearly flat bands. We then consider the superconducting phase and find that for different pairing symmetries, the numbers of bound states are different. Thus, it can serve as an indicator to show in which superconducting phase the TBG system is. The result can be summarized in the table below. Recently, STM experiments have successfully detected the local DOS of the TBG without impurities. There are some methods to introduce defects into the graphene, and the effect of defects can be then detected by STM experiments. We hope further STM results can determine the pairing symmetry of the superconducting TBG by examining the number of bound states.

When the strength or density of impurities is large, superconductivity in \((d+id)\)-wave phase and \((p+ip)\)-wave phase can be fully destroyed. This can also help us to determine whether the superconductivity in the TBG is conventional or unconventional.

V. ACKNOWLEDGEMENTS

HY and ZQG thank Ding-Ping Li, Xin-Zheng Li, Kai-Wei Sun and Shuai Wang for enlightening discussions. ZQG also thanks Ji-Chen Feng for helpful advice in some technical details. FW acknowledges support from The
VI. APPENDIX

Appendix A: Impurity Scattering Vertices

When taking account of superconductivity, we convert the impurity Hamiltonian we construct above to diagonal basis. Define

\[
U_{kk'}^{AB} = C_k \cdot u \left( T_{NN} \cdot J_{kk'}^{*}, T_{NN} \cdot J_{kk'}^{*} \right) \cdot C_k^{-1}, \quad (A1)
\]

\[
U_{kk'}^{BA} = C_k \cdot u \left( T_{NN} \cdot J_{kk'}^{*}, T_{NN} \cdot J_{kk'}^{*} \right) \cdot C_k^{-1}, \quad (A2)
\]

\[
U_{kk'}^{AA} = C_k \cdot M_{kk'} \cdot C_k^{-1}, \quad (A3)
\]

where

\[
M_{kk'} = u \left( t_{NN}^{A} \cdot J_{kk'}^{*} \cdot J_{kk'}^{*} \cdot t_{NN}^{A}, t_{NN}^{A} \cdot J_{kk'}^{*} \cdot J_{kk'}^{*} \cdot t_{NN}^{A}, t_{NN}^{A} \cdot J_{kk'}^{*} \cdot J_{kk'}^{*} \cdot t_{NN}^{A} \right)
\]

and \( C_k \) is the transform matrix between Wannier basis and diagonal basis.

Appendix B: Explanation for an Anomalous Feature of Some Figures

FIG. 12. Bogoliubov bands with and without superconductivity. In our choice of coefficients, because of the form factor of \((p + ip)\)-wave and \((d + id)\)-wave paring, the superconducting gap is comparable with the band gap at \( K \), as illustrated in the upper half of FIG. 12. For \( s \)-wave paring, the superconducting gap is always much smaller than the band gap at \( K \) as illustrated in the lower half of FIG. 12. Therefore, for \( s \)-wave phase, the local DOS of two gap edges have particle-hole symmetry in strength.

Some figures of local DOS in FIG. 6 and FIG. 7 show an anomalous feature, that for \((d + id)\)-wave phase and \((p + ip)\)-wave phase, the local DOS of two gap edges seemingly lose particle-hole symmetry in strength. Indeed, since under our choice of coefficients, the value of superconductor gap is comparable with Bogoliubov band gap at \( K \) point in the Brillouin zone, as shown in FIG. 12. However, particle-hole symmetry of the strength of the local DOS of two gap edges only occurs when the value of superconducting gap is much smaller than that of band gaps. Therefore, nothing will guarantee the particle-hole symmetry of the strength of the two gap edges in the DOS of \((d + id)\)-wave phase and \((p + ip)\)-wave phase in our model.
20. C.-C. Liu, L.-D. Zhang, W.-Q. Chen, and F. Yang, Phys. Rev. Lett. 121, 217001 (2018).

21. P. A. Lee and T. V. Ramakrishnan, Rev. Mod. Phys. 57, 287 (1985).

22. Y. Xie, B. Lian, B. Jck, X. Liu, C.-L. Chiu, K. Watanabe, T. Taniguchi, B. A. Bernevig, and A. Yazdani, Nature 572, 101 (2019).

23. A. Kerelsky, L. J. McGilly, D. M. Kennes, L. Xian, M. Yankowitz, S. Chen, K. Watanabe, T. Taniguchi, J. Hone, C. Dean, A. Rubio, and A. N. Pasupathy, Nature 572, 95 (2019).

24. Y. Jiang, X. Lai, K. Watanabe, T. Taniguchi, K. Haule, J. Mao, and E. Y. Andrei, Nature (2019), 10.1038/s41586-019-1460-4.

25. Y. Choi, J. Kemmer, Y. Peng, A. Thomson, H. Arora, R. Polski, Y. Zhang, H. Ren, J. Alicea, G. Refael, F. von Oppen, K. Watanabe, T. Taniguchi, and S. Nadj-Perge, arXiv e-prints, arXiv:1901.02997 (2019), arXiv:1901.02997 [cond-mat.mes-hall].

26. P. Ahlberg, F. O. L. Johansson, Z.-B. Zhang, U. Jansson, S.-L. Zhang, A. Lindblad, and T. Nyberg, APL Materials 4, 046104 (2016), https://doi.org/10.1063/1.4945587.

27. H. Gonzalez-Herrero, J. M. Gomez-Rodriguez, P. Mallet, M. Moaied, J. J. Palacios, C. Salgado, M. M. Ugeda, J.-Y. Veuillen, F. Yndurain, and I. Brihuega, Science 352, 437 (2016).