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Singlet superconductivity enhanced by charge order in nested twisted bilayer graphene Fermi surfaces

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ABSTRACT

Using the continuum model for low energy non-interacting electronic structure of moiré van der Waals heterostructures developed by Bistritzer and MacDonald [1], we study the competition between spin, charge, and superconducting order in twisted bilayer graphene. Surprisingly, we find that for a range of small angles inclusive of the so-called magic angle, this model features robust Fermi pockets that preclude any Mott insulating phase at weak coupling. However, a Fermi surface reconstruction at $\theta \gtrsim 1.2^{\circ}$ gives emergent van Hove singularities without any Fermi pockets. Using a hot-spot model for Fermi surface patches around these emergent saddle points, we develop a random-phase approximation from which we obtain a phase diagram very similar to that obtained recently by Isobe, Yuan, and Fu using the parquet renormalization group [2] but with additional insights. For example, our model shows strong nesting around time-reversal symmetric points at a moderate doping of $\sim 2 \times 10^{11}\,\mathrm{cm}^{-2}$ away from the van Hove singularity. When this nesting dominates, we predict that charge-order enhances singlet superconductivity, while spin-order suppresses superconductivity. Our theory also provides additional possibilities for the case of unnested Fermi surfaces.

1. Introduction

Recently, superconductivity (SC) and correlated insulating phases have been reported in twisted bilayer graphene (tBG) at small twist angles [3,4]. The insulating gap was observed when the first electron moiré band is half-filled with two electrons (or holes) per moiré unit cell. This is unexpected from the non-interacting picture, where the insulating phase occurs only when the first moiré band is completely filled and arises from the avoided crossing between the first and second moiré bands [5]. The superconductivity was observed at slight doping ($\sim 10^{11}\,\mathrm{cm}^{-2}$) away from the half-filled moiré band. The strong resemblance between the observed phase diagram in tBG and that of high-T_c cuprate and pnictide superconductors raises the tantalizing possibility that they share the same underlying mechanism. If true, then the relative theoretical simplicity of tBG (nothing more than two rotated sheets of carbon), as well as the relative ease to prepare and manipulate experimental samples, makes this an unprecedented platform to probe and understand high-T_c superconductivity. In recent weeks, there have been a flurry of theoretical efforts that attempt to understand the correlated phenomenon in this system including Refs. [2,6–20]. However, it is fair to say that the nature of the insulating phase, and the symmetry and mechanism of the superconducting pairing is still very much under debate.

The emergence of SC and insulating phases can be understood either from a strong coupling picture or at weak coupling. At strong coupling, an antiferromagnetic Mott insulating phase arises for Dirac fermions at charge neutrality from the short-range part of the Coulomb interaction (which is enhanced in tBG compared to monolayer graphene) [21]. Away from charge neutrality and at the half-filled moiré band, the SC can be understood as an emergent anti-ferromagnetic Heisenberg model where the pairing mechanism in the SC channel appears within mean field theory through a Fierz identity [6]. In the weak coupling theories (see e.g. Refs. [2,16,18]), the instability is due to the saddle points and near nesting of the non-interacting Fermi surface (FS). The strong particle-hole (p-h) fluctuation resulting from saddle points and FS nesting leads to density wave instabilities, which are predicted to be responsible for the insulating phase observed in experiment. The p-h fluctuations can also pair two electrons together to form SC. Since the non-interacting band-structure is known (see e.g. Ref. [1] and references therein), we focus here on weak coupling, while cognizant that a

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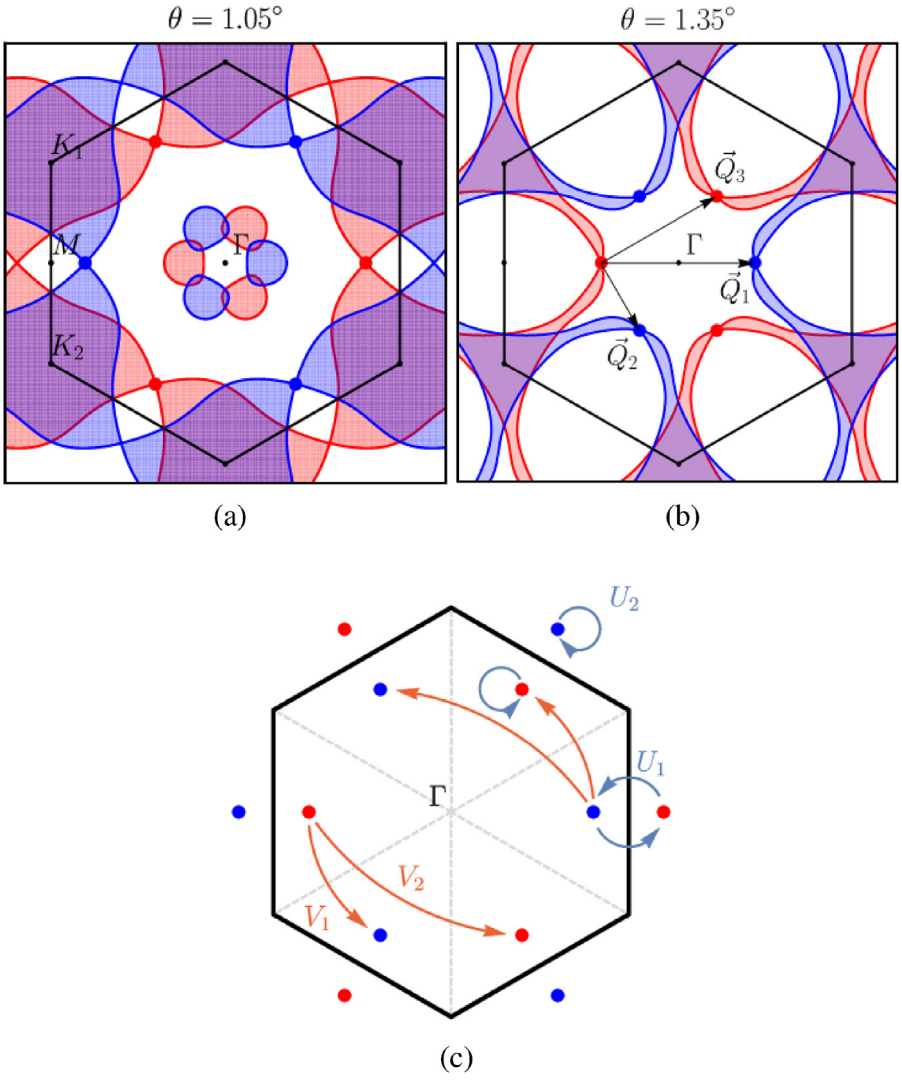

Fig. 1. Fermi surface reconstruction as a function of angle for twisted bilayer graphene. (a) The Fermi surface of the so-called "magic angle" of $\theta = 1.05^\circ$ when doped to the Van Hove energy. There are robust Fermi pockets close to the moiré Brillouin zone center. No nesting is observed for these Fermi pockets, and they are expected to remain gapless at weak coupling. Accordingly, no Mott insulating phase should be observed at this twist angle and chemical potential. (b) Fermi surface at twist angle $\theta = 1.35^\circ$ also at the Van Hove energy. At this angle the Fermi surface has a different topology with the Fermi pockets having merged with the saddle points. In this case, the weak coupling theory for twisted bilayer graphene is determined solely by the intra- and inter-saddle point couplings shown in (c). Here U_1 is the exchange interaction between the saddle point and its time-reversal partner, U_2 is the density-density interaction. V_1 and V_2 are the exchange interactions between two saddle points separated by $\vec{q} = \vec{Q}_2$ and $\vec{Q}_3$ marked in panel (b).

strong coupling mechanism could be operational in the experiments.

In this work, we study the Fermi surface topology using the Bistritzer and MacDonald continuum low energy model. At $\theta = 1.05^\circ$, we find robust non-nested Fermi pockets around Brillouin zone center when the chemical potential crosses saddle points. Based on this finding, we predict that no insulating phase should be observed at magic angle $\theta = 1.05^\circ$ in the weak coupling limit. To study the insulating and superconducting phases, we construct a hot-spot RPA model. If the Fermi surface is nested – as is widely believed – we predict that the insulating phase is charge-ordered and the superconductivity is a spin-singlet. Our model also allows us to explore other possibilities when the Fermi surface is not nested.

2. Model

2.1. Fermi surface of non-interacting bands

Interlayer coupling between TBG layers results in a hybridization between the Dirac bands which belong to the constituent layer. The essential features of the hybridized bands can be captured by three Fourier components of similar magnitude w, consistent with the underlying three-fold rotational symmetry of the tBG [1,22]. Our non-interacting model of tBG is fully based on the continuum model of Ref. [1], in which the Hamiltonian takes the following form:

$$H_s\left(\vec{k}_1, \vec{k}_2; \theta\right) = \begin{pmatrix} h_s\left(\vec{k}_1; \frac{\theta}{2}\right) & T_s(\vec{r}) \\ T_s^\dagger(\vec{r}) & h_s\left(\vec{k}_2; -\frac{\theta}{2}\right) \end{pmatrix}, \tag{1}$$

where $\vec{k}_1$ ($\vec{k}_2$) refers to the momentum states of the first (second) layer, while $s = \pm$ denotes the valley K/K'. We use the following convention in our work:

$$h_s\left(\vec{k}, \theta\right) = s v_F k \begin{pmatrix} 0 & e^{-is\left(\theta+\theta_{\vec{k}}\right)} \\ e^{is\left(\theta+\theta_{\vec{k}}\right)} & 0 \end{pmatrix}, \tag{2a}$$

$$T_s(\vec{r}) = w \sum_n \exp(-is\vec{q}_n \cdot \vec{r}) \begin{pmatrix} e^{i\frac{2ns\pi}{3}} & 1 \\ e^{-i\frac{2ns\pi}{3}} & e^{i\frac{2ns\pi}{3}} \end{pmatrix}, \tag{2b}$$

where v_F is the Fermi velocity of monolayer graphene, and $n \in \{0, 1, 2\}$. The vectors $\vec{q}_n = 2K \sin\left(\frac{\theta}{2}\right)\left[\mathscr{R}\left(\frac{2n\pi}{3}\right)\{0, 1\}\right]$ define the connections between momenta on different layers, i.e. $\vec{k}_2 = \vec{k}_1 + s\vec{q}_n$ and $\mathscr{R}(\phi)$ is the rotation operator. In our calculations, for the single adjustable parameter, we use the accepted value of $w = 110$ meV.

Under the influence of interlayer couplings, the bands experience significant reconstruction, such as avoided crossings at momentum states located midway between the Dirac points, Van Hove singularities (VHS) in the low-energy spectrum and Fermi velocity renormalization (see e.g. Ref. [5] and references therein). Interestingly, the