Effect of superconductivity on the shape of flat bands

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For the first time, basing both on experimental facts and our theoretical consideration, we show that Fermi systems with flat bands should be tuned with the superconducting state. Experimental measurements on magic-angle twisted bilayer graphene of the Fermi velocity $V_F$ as a function of the temperature $T_c$ of superconducting phase transition have revealed $V_F \propto T_c \propto 1/N_s(0)$, where $N_s(0)$ is the density of states at the Fermi level. We show that the high-$T_c$ compounds Bi$_2$Sr$_2$CaCu$_2$O$_{8+x}$ exhibit the same behavior. Such observation is a challenge to theories of high-$T_c$ superconductivity, since $V_F$ is negatively correlated with $T_c$, for $T_c \propto 1/V_F \propto N_s(0)$. We show that the theoretical idea of forming flat bands in strongly correlated Fermi systems can explain this behavior and other experimental data collected on both Bi$_2$Sr$_2$CaCu$_2$O$_{8+x}$ and twisted bilayer graphene. Our findings place stringent constraints on theories describing the nature of high-$T_c$ superconductivity and the deformation of flat band by the superconducting phase transition.

PACS numbers: 71.27.+a, 71.10.Hf, 74.70.Tx

INTRODUCTION

Recent experimental data revealed that in the superconducting state (SC) the dispersionless flat band vanishes, possessing a finite Fermi velocity $V_F$, $V_F \propto T_c$ [1]. This observation is in contrast with commonly accepted theoretical considerations, since $V_F$ is always negatively correlated with the superconducting phase transition temperature $T_c$ [1]. Thus, the experimental fact represents a challenging problem for the corresponding theory. Such a behavior is typical of Fermi systems with fermion condensation (FC) [2], and was predicted about twenty years ago [3]. The reason is that Fermi systems with flat bands should be tuned with the superconducting state: The dispersionless flat band vanishes, the effective mass $M^*$ becomes finite and the corresponding Fermi velocity $V_F = p_F/M^* \propto T_c \propto \Delta$, with $p_F$ and $\Delta$ being the Fermi momentum and the superconducting gap, respectively. Flat bands in Fermi systems with strong interaction were predicted about thirty years ago [4], and the properties of such systems are predicted and described in details, see e.g. [2, 5–13]. Topological approach turns out to be a powerful method to gain information about a wide class of physical systems. Understanding the topological properties allows one to augment the general knowledge about physical systems without solving specific equations. The microscopic approach to a heavy fermion (HF) metal (for example, computer simulations) gives only particular information about a specific many-body system, but not about the universal features, inherent in wide class of HF compounds [2, 9, 10].

HF compounds can be viewed as a new state of matter, since their behavior near the topological fermion condensation quantum phase transition (FCQPT) acquire important similarities in their thermodynamic and transport properties, making HF compounds a universal state of matter. The concept of FCQPT, forming the recent experimentally discovered flat bands, originated long ago [4]. At first, this idea appeared as a mathematical curiosity, but now the fermion condensation theory, based on FCQPT, represents an expanding field with numerous applications [2, 5–13]. Flat bands have been discovered experimentally in magic angle twisted bilayer graphene (MATBG). Namely, at a magic twist angle graphene transforms from a weakly correlated Landau Fermi liquid (LFL) to a strongly correlated two-dimensional electron system [14–18]. The flat band is driven by FCQPT and accompanied by FC transforming the Fermi surface into the Fermi volume, as depicted in Fig. 1 (a). This flat band becomes highly susceptible to reconstruction induced by external and internal factors such as magnetic field $B$, temperature $T$, including the setting in of phase transitions like antiferromagnetic, SC, etc, see e.g. [2, 5, 9–11]. In case of the flat band, the gap $\Delta$ depends linearly on the pairing interaction constant $g$, $\Delta \propto g$, see e.g. [2, 4, 5, 9–11, 19, 20].

The physics of high-$T_c$ superconductors (HTS), being the mainstream topic for more than thirty years, still seems to be elusive, and the mechanism of superconductivity in MATBG is constantly being debated, see e.g. [21]. Based on recent experimental measurements on MATBG with flat band [1] and FCQPT, we arrive at the conclusive statements about the underlying physics of HTS: Data collected on very different strongly correlated Fermi systems as Bi$_2$Sr$_2$CaCu$_2$O$_{8+x}$ and MATBG show that the Fermi velocity $V_F$ is proportional to the transition temperature $T_c$, $V_F \propto T_c$ [1, 22]. Taking into account that if pairing is mediated by phonons, or other bosons that are independent of $V_F$, one has that the density of states (DOS), $N_s(0) \propto 1/V_F \propto T_c$, see e.g. [1, 23–25],
and we face a challenging problem to explain the experimental data. We consider MATBG within the framework of the model of a homogeneous HF liquid [2]. This model avoids the complications associated with the anisotropy of solids and considers both the thermodynamic properties and the non Fermi liquid (NFL) behavior by calculating the effective mass \( M^*(T, B) \) as a function of \( T \) and \( B \) [2, 10]. The model is applicable in our case, since \( V_F \approx 10^4 \text{ m/s} \) is a hundred or more times smaller than electron velocities of isolated graphene sheets [1]. Therefore, the wavelength of an electron is much larger than the distance between carbon atoms of the sheet; consequently, we can use the well-known jelly model [2].

In this Letter, for the first time, basing both on experimental facts [1, 22] and our theoretical consideration, we show that Fermi systems with flat bands should be tuned with the superconducting state: Flat, or approximately flat, band, possessing almost infinite effective mass \( M^* \), vanishes and the corresponding Fermi velocity becomes \( V_F = p_F/M^* \propto T_c \propto \Delta \). We demonstrate that such a behavior is a general property and experimentally observed in the HTS Bi_2Sr_2CaCu_2O_8+x and graphene. This behavior is in contrast to the standard case of BCS, or to other theories of HTS, where the single particle electron spectrum does not depend on \( \Delta \). We also recall that the thermodynamic properties of Fermi systems with flat bands generated by FC strongly depend on external parameters like \( T, B \), etc. Our findings place strong constraints on theories describing the high-\( T_c \) superconductivity.

**FLAT BAND AND SUPERCONDUCTING STATE**

We start with considering a Fermi system with FC at \( T = 0 \). We employ weak BCS-like interaction with the coupling constant \( g \) and analyze the behavior of both the superconducting gap \( \Delta \) and the superconducting order parameter \( \kappa(p) \) as \( g \to 0 \). Let us write the usual pair of equations for the Green’s functions \( F^+(p, \omega) \) and \( G(p, \omega) \) [25]

\[
F^+ = \frac{-i\Xi^*}{(\omega - E(p) + i0)(\omega + E(p) - i0)}, \tag{1}
\]

\[
G = \frac{u^2(p)}{\omega - E(p) + i0} + \frac{v^2(p)}{\omega + E(p) - i0}, \tag{2}
\]

where \( E^2(p) = \xi^2(p) + \Delta^2 \), \( \xi(p) = \varepsilon(p) - \mu \). Here, \( \varepsilon(p) \) is the single particle energy and \( \mu \) is the chemical potential. The gap \( \Delta \) and the function \( \Xi \) are given by

\[
\Delta = g|\Xi|, \quad i\Xi = \int F^+(p, \omega) \frac{d\omega d\mathbf{p}}{(2\pi)^4}. \tag{3}
\]

Here \( v^2(p) = (1 - \xi(p)/E(p))/2, v^2(p) + u^2(p) = 1 \), and simple algebra gives

\[
\xi(p) = \Delta \frac{1 - 2v^2(p)}{2\kappa(p)}, \tag{4}
\]

with \( \kappa(p) = u(p)v(p) \) being the superconducting order parameter [26]. It is directly seen from Eq. (4) that \( \xi \to 0 \) as soon as \( \Delta \to 0 \), provided that \( \kappa(p) \neq 0 \) in some region \( p_i < p < p_f \); thus, the band becomes flat in the region, since \( \varepsilon(p) = \mu [2, 3] \). Next, we observe from Eqs. (3) and (4) that

\[
i\Xi = \int_{-\infty}^{\infty} F^+(p, \omega) \frac{d\omega d\mathbf{p}}{(2\pi)^4} = i \int \kappa(p) \frac{d\mathbf{p}}{(2\pi)^3}. \tag{5}
\]

Clearly seen from Eqs. (3), (4) and (5) is that as \( g \to 0 \) the superconducting gap \( \Delta \to 0 \), while \( \xi = 0 \) and the dispersion \( \varepsilon(p) \) becomes flat. Then, \( \kappa(p) \) remains finite in some region \( p_i \leq p \leq p_f \), making \( \Xi \) finite. Thus, in the state with FC \( \Delta \) can vanish while the order parameters \( \kappa(p) \) and \( \Xi \) are finite. Taking into account Eqs. (3) and (4) we transform Eqs. (1) and (2) as follows

\[
F^+ = -\frac{\kappa(p)}{\omega - E(p) + i0} + \frac{\kappa(p)}{\omega + E(p) - i0}, \tag{6}
\]

\[
G = \frac{u^2(p)}{\omega - E(p) + i0} + \frac{v^2(p)}{\omega + E(p) - i0}. \tag{7}
\]

Here, at the region \( p_i \leq p \leq p_f \), occupied by FC, the factors \( v^2(p), u^2(p) = 1 - v^2(p), v(p)u(p) = \kappa(p) \neq 0 \) are determined by the condition \( \varepsilon(p) = \mu \), while \( E(p) \to 0 [2, 4, 5] \). From Eqs. (6) and (7) it is seen that in the FC state as \( g \to 0 \), the equations for \( F^+(p, \omega) \) and \( G(p, \omega) \) take the following form in the FC region

\[
F^+(p, \omega) = -\kappa(p) \left[ \frac{1}{\omega + i0} - \frac{1}{\omega - i0} \right], \tag{8}
\]

\[
G(p, \omega) = \frac{u^2(p)}{\omega + i0} + \frac{v^2(p)}{\omega - i0}. \tag{9}
\]

Upon integrating \( G(p, \omega) \) over \( \omega \) we obtain that \( v^2(p) = n(p) \), where \( n(p) \) is the quasiparticles distribution function. From Eq. (3) \( \Delta \) is seen to be a linear function of the coupling constant \( g \) [4, 19, 20]. Since the transition temperature \( T_c \sim \Delta \) tends to zero along with \( g \to 0 \), the order parameter \( \kappa(p) \) of the FC state vanishes at finite temperatures via the first order phase transition [27]. Thus, a flat band represents a special solution of the BSC equations. In contrast to BSC-like theories, Eq. (4) defines the dependence of spectrum \( \xi \) on \( \Delta \), and, as we will see below, leads to \( V_F \propto T_c [1–3] \).

At finite \( T > 0 \) the quasiparticle occupation number is given by the Fermi-Dirac distribution function which is represented in the form [5]

\[
\varepsilon(p, T) - \mu(T) = T \ln(1 - n_0(p, T))/n_0(p, T). \tag{10}
\]
FIG. 1: Flat band induced by FC. (a) The flat single particle spectrum with \( V_F = 0 \) at \( T = 0 \) is shown by the solid curve. The changed flat band with the emergence of the SC state with finite \( V_F \) is shown by the dashed line, see Eq. (13). This change is depicted by the arrow, and is schematically shown by the solid and dashed lines. The dashed area displays the flat band deformed by the superconducting state. Insert: The quasiparticle occupation number, \( n(k) \) at \( T = 0 \) versus the dimensionless momentum \( k = p/p_F \), where \( p_F \) is the Fermi momentum. (b): The single particle spectrum \( \epsilon(k,T) \) at \( T/E_F \); temperature is measured in the units of \( E_F \). (c) The distribution function \( n(k,T) \) is asymmetric with respect to the Fermi level \( E_F \), generating specific NFL behavior and causing the breakdown of both C- and T-invariance. To clarify the asymmetry, the area occupied by holes in panel (b) is marked by letter "h", while that for quasiparticles is marked by "p".

Observing that as \( T \rightarrow 0 \), the distribution function satisfies the inequality \( 0 < n_0(p) < 1 \) for \( p_i \leq p \leq p_f \), we see that the logarithm is finite and, therefore, the right hand side of Eq. (10) vanishes. Taking into account the well-known Landau equation \( \frac{\delta E[n(p)]}{\delta n(p)} = \epsilon(p) = \mu \); \( p_i \leq p \leq p_f \), we conclude that at \( T = 0 \) Eq. (11) determines \( n_0(p) \) [4]

\[
\frac{\delta E[n(p)]}{\delta n(p)} = \epsilon(p) = \mu; \quad p_i \leq p \leq p_f,
\]

where \( E[n(p)] \) is the Landau functional [25]. Being exact [28] and in accordance with Eq. (4), Eq. (11) describes the state with FC characterized by the superconducting order parameter \( \kappa_0(p) = \sqrt{n_0(p)(1 - n_0(p))} \) where the functions \( n_0(p) \) are solutions of Eq. (11). It is instructive to construct \( F^+(p,\omega) \) and \( G(p,\omega) \) when \( g \) is finite but small so that the functions \( v^2(p) \) and \( \kappa(p) \) can be approximated by the solutions of Eq. (11). In that case, \( \Xi, \Delta \) and \( E(p) \) are given by Eqs. (5), (3) and (4) respectively. Inserting these into Eqs. (6) and (7), we obtain the functions \( F^+(p,\omega) \) and \( G(p,\omega) \).

Let us use Eq. (4) to calculate \( M^* \) by differentiating both sides of this equation with respect to the momentum \( p \) at \( p = p_F \). Then

\[
M^* \simeq p_F \frac{p_f - p_i}{2\Delta}.
\]

When obtaining Eq. (12), we took into account that \( \kappa(p) = 1/2 \) at \( p = p_F \), the gap \( \Delta(p) \) has a maximum value \( \Delta_0 \) at the Fermi surface, and, hence, its derivative there equals zero. The derivative \( d(n(p))^2/dp \) was calculated using the simple estimate \( dn(p)/dp \simeq 1/(p_f - p_i) \). Since from Eq. (12) \( V_F \propto T_c \propto \Delta \), therefore

\[
V_F \simeq 2\Delta \frac{p_f - p_i}{p_f - p_i} \propto T_c.
\]

From Eq. (13) as \( T_c \rightarrow 0 \), the Fermi velocity \( V_F \rightarrow 0 \) and the band becomes exactly flat representing a plateau. When \( T_c \) is finite the plateau is slightly tilted and rounded off at its end points, as shown in Fig. 1. At increasing \( \Delta \propto T_c \), both \( M^* \) and DOS are reduced and \( V_F \) grows. Thus, the electronic system with FC in the superconducting state is characterized by two effective masses: \( M^* \) is the effective mass given by Eq. (12) and related to the area \( (p_f - p_i) \), with the effective mass \( M^*_L \) located at \( p \lesssim p_i \) [2]. Seen from Fig. 1 (a) is that the plateau of the flat band of the SC system with FC is slightly tilted and \( M^* \) becomes finite. Indeed, from Eq. (13) \( V_F \propto \Delta \propto T_c \), while at \( T \leq T_c \) the Fermi velocity \( V_F \) does not depend on temperature [2, 3, 9, 10]. At \( T \simeq T_c \) and under the application of magnetic field, the superconducting phase transition is of second order, therefore, the single-particle spectrum is not changed and \( M^* \) does not change at \( T \simeq T_c \). Thus, at \( T \simeq T_c \), Eq. (13) is valid, for \( M^* \) coincides in the superconducting state and normal states [1, 2]. At \( T > T_c \) the slope of the flat band is proportional to \( T_c \), as seen from Fig. 1 (b). For example, such a dependence can be measured by using ARPES. Note that the single particle spectrum of a system with FC is sensitive to the state of the system in question, and changes with the application of external parameters like pressure, magnetic field, temperature, etc. [2, 9, 10]. It is also seen from Fig. 1 (b) that both the particle - hole symmetry C and the time invariance T are violated resulting in the asymmetrical differential tunneling conductivity, and being suppressed in magnetic fields that
drive the system to its LFL state. This behavior has been predicted and evaluated [2, 29, 30], and turns out to be consistent with the experimental facts [14, 22, 31–33].

Measurements of $V_F$ and $N_s(0)$ versus $T_c$ [1] are displayed in Figs. 2 (a) and (b) and taken from Refs [1, 22, 34–37]. The inset in Fig. 2 (b) shows experimental facts collected on the HTS Bi$_2$Sr$_2$CaCu$_2$O$_{8+x}$, with $x$ is oxygen doping concentration [22]. The local density of states (LDOS) is shown in arbitrary units (au), the straight line depicts that LDOS is inversely proportional to $\Delta$. It is seen from the inset that the data taken at the position with the highest integrated LDOS has the smallest gap value $\Delta$ [22]. These observations in accordance with Eqs. (12) and Eq. (13). Thus, our theoretical prediction [2, 3] agrees very well with the experimental results [1, 22]. It is noted that $V_F \to 0$ as $T_c \to 0$, seen from Figs. 2. This result demonstrates that the flat band is disturbed at finite $\Delta$, and possesses a finite slope, as seen from Fig. 1 (a). Clearly, from Figs. 2, the experimental critical temperature $T_c$ does not correspond to the Fermi velocity $V_F$ minima as they would in any theory wherein pairing is mediated by phonons (bosons) that are insensitive to $V_F$ [1]. Thus, such behavior is in contrary to that expected within the framework of the common BSC-like theories that do not assume that the single particle spectra strongly depend on the pairing correlations [1, 2, 23, 24]. This behavior is based on the topological FCQPT forming flat bands [2, 3, 9, 10]. We note that in case of graphene a flat band can be disturbed by some external parameters like the critical angle at which the flat band is emerged. In that case Eq. (13) is valid at relatively high values of $\Delta$ that disturb the flat band more strongly than the external parameters [2]. Bi$_2$Sr$_2$CaCu$_2$O$_{8+x}$ exhibits this behavior shown in the inset to Fig. 2 (b).

We now consider briefly the entropy $S(T)$ of the system under consideration, given by the well-known expression [25]

$$S = -2 \int [n_0 \ln n_0 + (1 - n_0) \ln(1 - n_0)] \frac{dP}{(2\pi)^3}. \tag{14}$$

The entropy $S$ in Eq. (14), as the special solution $n_0(\mathbf{p})$ of Eq. (11), contains the temperature independent term $S_0 = S(T \to 0) \sim (p_f - p_n)/p_F$. Thus, the function $n_0(\mathbf{p})$ representing the special solutions of both BCS and LFL equations determines the NFL behavior. Namely, contrary to conventional BCS case, the FC solutions are characterized by infinitesimal value of the superconducting gap, $\Delta \to 0$, while both $\kappa(\mathbf{p})$ and $\Xi$ remain finite and $S = 0$. In contrast to the usual solutions of the LFL theory, the special solution $n_0(\mathbf{p})$ is characterized by the entropy $S$ containing the temperature independent term $S_0$. As $T \to 0$ both the normal state of the HF liquid with the finite entropy $S_0$ and the BCS state with $S = 0$ coexist being separated by the first order quantum phase transition represented by the topological FCQPT, at which the Fermi surface transforms into the Fermi volume, forming a new quantum liquid [6]. At this first order phase transition the entropy undergoes a finite jump $\delta S = S_0$. Because of the thermodynamic inequality, $\delta Q \leq T \delta S$, the heat $\delta Q$ of the transition is equal to zero making the other thermodynamic functions continuous. Thus, at the topological FCQPT there are no strong critical fluctuations accompanying second order phase transitions and suppressing the quasiparticles. Therefore, the quasiparticles survive and define the thermodynamic and transport properties of HF compounds [2, 5, 8, 9], rather than quantum critical fluctuations, see e.g [38].

![FIG. 2: Experimental results for the average Fermi velocity $V_F$ versus the critical temperature $T_c$ for MATBG. The results are taken from [1]. (a) Experiment is shown by the squares [1], the square marked by the arrow represents experiment [34]. (b) Experiment is shown by the stars [1, 35–37]. Theory is displayed by the solid line. Inset is adopted from [22], and depicts experimental dependence of the superconducting gap versus the local density of states (LDOS) collected on the HTS Bi$_2$Sr$_2$CaCu$_2$O$_{8+x}$; $x$ is oxygen doping concentration.](image-url)
SUMMARY

The main message of our Letter is that Fermi systems with flat bands should be tuned with the superconducting state so that Fermi velocity $V_F = p_F/M^* \propto 1/N_s(0) \propto T_c \propto \Delta$. Such a correlation of the properties of the flat band Fermi systems with the superconducting state is a new universal effect and it has been observed recently in graphene [1] as well as in the high $T_c$ superconductors $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x}$ [22] that are completely different by their microscopic structures. The data are well explained in the framework of fermion condensation theory and to our best knowledge there is no any other standard theoretical framework that can do the same, since the BCS like theories state $T_c \propto N_s(0)$ [1, 23–25]. Finally, our study of the experimental results [1, 22] confirms that the topological FCQPT is the intrinsic feature of many strongly correlated Fermi systems and can be viewed as the universal cause of both the NFL behavior and the corresponding new state of matter [10].

We thank V. A. Khodel for fruitful discussions. This work was partly supported by U.S. DOE, Division of Chemical Sciences, Office of Basic Energy Sciences, Office of Energy. This work is partly supported by the RFBR No. 19-02-00237.

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