The influence of topological phase transition on the superfluid density of overdoped copper oxides

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We show that a topological quantum phase transition, generating flat bands and altering Fermi surface topology, is a primary reason for the exotic behavior of the overdoped high-temperature superconductors represented by La2−xSrxCuO4, whose superconductivity features differ from what is described by the classical Bardeen-Cooper-Schrieffer theory [J.I. Božović, X. He, J. Wu, and A. T. Bollinger, Nature 536, 309 (2016)]. We demonstrate that 1) at temperature $T = 0$, the superfluid density $n_s$ turns out to be considerably smaller than the total electron density; 2) the critical temperature $T_c$ is controlled by $n_s$ rather than by doping, and is a linear function of the $n_s$; 3) at $T > T_c$, the resistivity $\rho(T)$ varies linearly with temperature, $\rho(T) \propto \alpha T$, where $\alpha$ diminishes with $T_c \to 0$, while in the normal overdoped (non superconducting) region with $T_c = 0$, the resistivity becomes $\rho(T) \propto T^2$. The theoretical results presented are in good agreement with recent experimental observations, closing the colossal gap between these empirical findings and Bardeen-Cooper-Schrieffer-like theories.

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I. INTRODUCTION

By now, overdoped copper oxides are realized as simple HTSC, whose strongly correlated physics can be captured by the conventional Bardeen-Cooper-Schrieffer theory (BCS), while recent experimental studies of overdoped high-$T_c$ superconductors (HTSC) La2−xSrxCuO4 discovered strong deviations of their physical properties from those predicted by BCS theory1,2. These deviations were surprisingly similar for numerous HTSC samples1–6. The measurements of the absolute values of the magnetic penetration depth $\lambda$ and the phase stiffness $\rho_s = A/\lambda^2$ were carried out on thousands of perfect two dimensional (2D) samples of La2−xSrxCuO4 (LSCO) as a function of the doping $x$ and temperature $T$. Here $A = d^{4}/4k_{B}e^{2}$ where $d$ is the film thickness, $k_B$ is Boltzmann constant, and $e$ is the electron charge. It has been observed that the dependence of zero-temperature superfluid density (the density of superconductive electrons) $n_s = 4\rho_s k_B m^*$ ($m^*$ is the electron effective mass), is proportional to the critical temperature $T_c$ over a wide doping range. This dependence coincides with perruous measurements, and is incompatible with the standard BCS description. Moreover, $n_s$ turns out to be considerably smaller than the BCS density $n_{el}$ of superconductive electrons1–6, which is approximately equal to the total electron density7. These observations representing the intrinsic LSCO properties provide unique opportunities for checking and expanding our understanding of the physical mechanisms responsible for high-$T_c$ superconductivity. We note, that that knowing the responsible mechanism can open avenue for chemical preparation of high-$T_c$ materials with $T_c$ as high as room temperature8–12.

Here we show that the physical mechanism, responsible for above non-BCS behavior of overdoped LSCO, stems from the topological fermion condensation quantum phase transition (FCQPT) accompanied by so-called fermion condensation (FC) phenomenon generating flat bands8–14. We note that flat bands and extended saddle point singularity play important role in the theory of HTSC, see e.g. Refs.12–16.

In order to make our analysis of overdoped LSCO obvious, we use the model of homogeneous heavy-electron liquid9,14. The main experimental facts of Refs.1,2 represent vivid qualitative deviations from those predicted by the classical BCS theory, therefore as a first step, we can confine ourselves to obtaining transparent analytical results describing quantitatively experimental facts. Our analysis shows that despite drastic microscopic diversity of strongly correlated Fermi systems, they exhibit similar behavior close to FC quantum phase transition point. This is actually related to the altering of Fermi surface topology during FCQPT. We emphasize that the quantum physics of all seemingly different strongly correlated Fermi systems (and overdoped HTSC among them) is universal and emerges regardless of their underlying microscopic details like the symmetries of their crystal lattices. Because we deal effectively with momenta transfers that are small compared to those of the order of the reciprocal lattice length (Brillouin zone boundaries), whose contributions have no effect on the topological properties of the systems under consideration9,12,14. Note that despite the highly anisotropic electronic band dispersion in overdoped cuprate HTSC and hence their Fermi surface, our theory still applies for this case. The point here is that after FCQPT the Fermi surface, regardless its initial anisotropy, changes its topological class, thus generating all aforementioned salient experimentally observed features, inherent in the fermion condensation state. In other words, any initially (highly) anisotropic Fermi sur-
face is still homotopic to simply spherical one as they can be reduced to each other by continuous deformation\textsuperscript{17,18}. In the superconducting state, to the first approximation different regions with the maximal absolute value of the $d$-wave superconducting order parameter are disconnected. Therefore, the order parameter can be either even, or odd with respect to a $\pi/2$ rotation in the ab-plane\textsuperscript{15,16}. Thus, as a first step, we also neglect the $d$-wave symmetry of the superconducting order parameter and use the s-wave one.

In our paper, using formalism accounting for the FC-QPT, we investigate overdoped LSCO and show that as soon as the doping $x$ reaches its FCQPT critical value $x_c$, the features of the emergent superconductivity begin to differ from those of BCS theory, as it is predicted long before the experimental observations are obtained\textsuperscript{1,2,19}. We demonstrate that: i) at $T = 0$, the superfluid density $n_s$ turns out to be a small fraction of the total density of electrons; ii) the critical temperature $T_c$ is controlled by $n_s$ rather than by doping, and is a linear function of the $n_s$. Since FCQPT generates flat electronic bands\textsuperscript{8–12}, the system under consideration exhibits non-Fermi liquid (NFL) behavior and the resistivity $\rho$ diminishes with $T$, being $\propto T^{\alpha}$ for $\alpha > 0$\textsuperscript{15,16}. Thus, as a first step, we also neglect the $d$-wave superconducting order parameter are disconnected. Therefore, the order parameter can be either even, or odd with respect to a $\pi/2$ rotation in the ab-plane\textsuperscript{15,16}. Thus, as a first step, we also neglect the $d$-wave symmetry of the superconducting order parameter and use the s-wave one.

At $T = 0$, the onset of FC in homogeneous matter is attributed to a nontrivial solution $n_0(p)$ of the variational equation\textsuperscript{8}

$$\frac{\delta E[n(p)]}{\delta n(p)} - \mu = 0, \quad p \in [p_i, p_f],$$

where $E$ is a ground state energy functional (its variation gives a single - electron spectrum $\epsilon$) and $p_i, p_f$ stand for initial and final momenta, where the solution of Eq. (3) exists, see Refs.\textsuperscript{5,9,14} for details. To be more specific, Eq. (3) describes a flat band pinned to the Fermi surface and related to FC.

To explain emergent superconductivity at $x \to x_c$, we retain the consequences of flattening of single-particle excitation spectra $\epsilon(p)$ (i.e. flat bands appearance) in strongly correlated Fermi systems, see Refs.\textsuperscript{5,12} for recent reviews. At $T = 0$, the ground state of a system with a flat band is degenerate, and the occupation numbers $n_0(p)$ of single-particle states belonging to the flat band are continuous functions of momentum $p$, in contrast to standard LFL “step” from 0 to 1 at $p = p_F$, as it is seen from Fig. 1. Thus at $T = 0$ the superconducting order parameter $\kappa(p) = \sqrt{n(p)(1 - n(p))} \neq 0$ in the region occupied by FC\textsuperscript{9,13,14,19,21}. This property is in a stark contrast to standard LFL picture, where at $T = 0$ and $p = p_F$ the order parameter $\kappa(p)$ is necessarily zero, see Fig. 1. Due to the fundamental difference between the FC single-particle spectrum and that of the remainder of the Fermi liquid, a system having FC is, in fact, a two-component system, separated from ordinary Fermi liquid by the topological phase transition\textsuperscript{11–13}. The range $L$ of momentum space adjacent to $\mu$ where FC resides is given by $L \simeq p_f - p_i$, see Fig. 1.

II. TWO-COMPONENT SYSTEM

An important problem for the condensed matter theory is the explanation of the NFL behavior observed in HTSC beyond critical point where the low-temperature density of states $N(T \to 0)$ diverges which can generate flat bands without breaking any ground state symmetry, see e.g. Refs.\textsuperscript{1,12,14,20–22}. In a homogeneous matter, such a divergence is associated with the onset of a topological transition at $x \to x_c$, signaled by the emergence of an inflection point at $p = p_F$\textsuperscript{13,14,23}

$$\epsilon - \mu \sim -(p_F - p)^2, \quad p < p_F, \quad (1)$$

$$\epsilon - \mu \sim (p - p_F)^2, \quad p > p_F, \quad (1)$$

at which the electron effective mass diverges as $m^*(T \to 0) \propto T^{-1/2}$, where $\epsilon$ is the single - electron energy spectrum, $p$ is a momentum, $p_F$ is Fermi momentum and $\mu$ is the chemical potential. Accordingly, at $x \to x_c$ the density of states diverges

$$N(T \to 0) \propto |\epsilon - \mu|^{-1/2}. \quad (2)$$

As a result, both FC state and the corresponding flat bands emerge beyond the topological FCQPT\textsuperscript{9,13,14,21}, while the critical temperature turns out to be $T_c \propto \sqrt{x - x_c}$\textsuperscript{15,16}. These results are consistent with the experimental data\textsuperscript{1}. The detailed consideration of this case will be published elsewhere.

III. GREEN FUNCTIONS AND SUPERFLUID DENSITY

To analyze the above emergent superconductivity quantitatively, it is convenient to use the formalism of Gor’kov equations for Green’s functions of a superconductor\textsuperscript{14,25,26}. For the 2D case of interest, the solutions of Gor’kov equations\textsuperscript{14,25,26} determine the Green’s functions $F^+(p, \omega)$ and $G(p, \omega)$ of a superconductor:

$$F^+(p, \omega) = \frac{-g_0 \Xi^*}{(\omega - E(p) + i0)(\omega + E(p) - i0)};$$

$$G(p, \omega) = \frac{u^2(p)}{\omega - E(p) + i0} + \frac{\bar{u}^2(p)}{\omega + E(p) - i0}. \quad (4)$$

Here the single-particle spectrum $\epsilon(p)$ is determined by Eq. (3), and

$$E(p) = \sqrt{\epsilon^2(p) + \Delta^2(p)}; \quad \frac{\Delta(p)}{E(p)} = 2\kappa(p). \quad (5)$$
satisfies the condition

\[ \varepsilon(p) = \mu. \]

The gap \( \Delta \) and the function \( \Xi \) are given by

\[ \Delta = g_0|\Xi|, \quad i\Xi = \int F^+(p, \omega) \frac{d\omega dp}{(2\pi)^3}. \]  

(6)

Here \( g_0 \) is the superconducting coupling constant. We remember that the function \( F^+(p, \omega) \) has the meaning of the wave function of Cooper pairs and \( \Xi \) is the wave function of the motion of these pairs as a whole. Taking Eqs. (5) and (6) into account, we can rewrite Eqs. (4) as

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

(7)

In the case \( g_0 \to 0 \), the gap \( \Delta \to 0 \), but \( \Xi \) and \( \kappa(p) \) remain finite if the spectrum becomes flat, \( E(p) \to 0 \), and in the interval \( p_i \leq p \leq p_f \) Eqs. (7) become

\[
F^+(p, \omega) = -\kappa(p) \left[ \frac{1}{\omega + i0} - \frac{1}{\omega - i0} \right], \\
G(p, \omega) = \frac{u^2(p)}{\omega + i0} + \frac{v^2(p)}{\omega - i0}.  
\]

(8)

The parameters \( u(p) \) and \( v(p) \) are the coefficients of corresponding Bogolubov transformation\(^{25,26} \), \( u^2(p) = 1 - n(p) \), \( v^2(p) = n(p) \). They are determined by the condition that the spectrum should be flat: \( \varepsilon(p) = \mu. \) It follows from Eqs. (5) and (6) that

\[
i\Xi = \int F^+(p, \omega) \frac{d\omega dp}{(2\pi)^3} = i \int \kappa(p) \frac{dp}{(2\pi)^2} \simeq n_{FC}, \]

(9)

where \( n_{FC} \) is the density of superconducting electrons, forming the FC component, see Fig. 1.

We construct the functions \( F^+(p, \omega) \) and \( G(p, \omega) \) in the case where the constant \( g_0 \) is finite but small, such that \( \varepsilon(p) \) and \( \kappa(p) \) can be found from the FC solutions of Eq. (3). Then \( \Xi, \Delta \) and \( E(p) \) are given by Eqs. (9), (6) and (5), respectively. Substituting the functions constructed in this manner into (7), we obtain \( F^+(p, \omega) \) and \( G(p, \omega) \). We note that Eqs. (6) and (9) imply that the gap \( \Delta \) is a linear function of both \( g_0 \) and \( n_{FC} \). Since \( T_c \sim \Delta \), we conclude that \( T_c \propto n_{FC} \propto \rho_s \). Note that since we consider the overdoped HTSC case and FCQPT takes place at \( x = x_c, n_{FC} \propto \rho_{F} \propto \rho_s \) \( \propto (p_f - p_i)/p_f \ll 1^{14,19,24} \), therefore

\[
n_{FC} = n_s \ll n_{el}. \]

(10)

Increasing \( g_0 \) causes \( \Delta \) to become finite, leading to a finite value of the effective mass \( m_{FC}^* \) in the FC state\(^{14} \):

\[
m_{FC}^* \simeq \frac{p_f - p_i}{2\Delta}. \]

(11)

An important fact is to be noted here. Namely, it have been shown in Refs.\(^{9,14} \), that in the FC formalism, the BCS relations remain valid if we use the spectrum given by Eq. (11). Thus, we can use the standard BCS approximation with the momentum independence of superconducting coupling constant \( g_0 \) in the region \( |\varepsilon(p) - \mu| \ll \omega_D \) so that the interaction is supposed to be zero outside this region. Here \( \omega_D \) is a characteristic energy, proportional to the Debye temperature. Under these suppositions, the superconducting gap depends only on temperature and is determined by the equation\(^{9,13,14} \)

\[
\frac{1}{g_0} = N_{FC} \int_{0}^{E_0/2} \frac{d\xi}{f(\xi, \Delta)} \tanh \frac{f(\xi, \Delta)}{2T} + N_L \int_{E_{0}/2}^{\omega_D} \frac{d\xi}{f(\xi, \Delta)} \tanh \frac{f(\xi, \Delta)}{2T},  
\]

(12)

where \( f(\xi, \Delta) = \sqrt{\xi^2 + \Delta^2(T)} \) and \( E_0 = \varepsilon(p_f) - \varepsilon(p_i) \approx 2\Delta (T = 0) \) is a characteristic energy scale. Also, \( N_{FC} = (p_f - p_i)p_F/(2\pi\Delta(T = 0)) \) and \( N_L = m_1^*/(2\pi) \) \( m_1^* \) is the effective mass of electron of the LFL component, see Fig. 1) are the densities of states of FC and non-FC electrons respectively. In the opposite case \( T = 0 \), as usual, \( \tanh(f/(2T)) = 1 \) and the remaining integrals can be evaluated exactly. This yields following equation relating the value \( \Delta(T = 0) \) with superconducting coupling constant \( g_0 \)

\[
\frac{\delta}{\beta} = B - \delta \ln \delta, \]

(13)
in FC phase. As a result, we have that in latter phase \( n_s < n_{el} \) with \( n_s \) and \( n_L \) being, respectively, the total density of electrons and that out of FC phase. Note that the result \( n_s \sim n_{el} \) does not only follow from BCS theory of superconductivity, but is much deeper and is pertinent to almost any superfluid system, being the result of the Leggett theorem\(^{28}\). The short statement of latter theorem\(^{28}\) is that at \( T = 0 \) in any superfluid liquid \( n_s \sim n_{el} \), here \( n_{el} \) denotes the number density of the liquid particles. For this theorem to be true, however, the system should be T - invariant, where T relates to time reversal. Since FC state, being highly topologically nontrivial\(^{9,29,30}\) violates primarily the time reversal symmetry (actually it also violates the CP invariance, where C is charge conjugation and P is translation invariance, see Refs.\(^9,14,29\) for more details), the inequality \( n_s < n_{el} \) is inherent in it, as it is seen from Eqs. (9) and (10). This implies that the main contribution to the above superconductivity comes from the FC state. We conclude that in the FC case the emerging two-component system violates the BCS condition that \( n_s \approx n_{el} \).

### IV. Penetration Depth and General Properties

Now we find out if our superconductor belongs to the London type. For that, we write down London’s electrodynamics equations: \( \nabla \times \mathbf{j}_s = -(n_s e^2/m^*) \mathbf{B} = -(n_{FC} e^2/m_{FC}^*) \mathbf{B} \) and \( \nabla \times \mathbf{B} = 4 \pi \mathbf{j}_s \), where \( \mathbf{j}_s \) is a superconducting current. These equations imply that the penetration depth

\[
\lambda^2 = \frac{m_{FC}^*}{4 \pi e^2 n_{FC}}. \tag{14}
\]

Comparing the penetration depth (14) with the coherence length \( \xi_0 \sim p_F/(m_{FC}^* \Delta) \), we conclude that \( \lambda >> \xi_0 \) as the FC quasiparticle effective mass is huge\(^9\). Thus, the superconductors are indeed of the London type.

It turns out that in FC phase, the penetration depth is a function not only of temperature but also of doping degree \( x \). Then, it follows from Ginzburg-Landau theory, that the density of superconducting electrons \( n_s \sim T_c^{-1} \). On the other hand, as it has been discussed in the paper\(^1\), the pressure enhances \( n_s \), i.e. the density \( x \) of charge carriers is important. Also, it has been shown (see, e.g. Refs.\(^9,14\)) that in superconducting phase with FC \( T_c \approx 2 \Delta(T = 0) \). This permits to use the relation (14) to plot the penetration depth as a function of temperature and doping in the form

\[
\frac{\lambda}{\lambda_0} = \frac{1}{\sqrt{y - \tau}}, \tag{15}
\]

where \( y = (x_c - x)/x_c, \tau = T/(2 \Delta(T = 0) x_c) \) and \( \lambda_0 \) combines all proportionality coefficients entering the problem. The dependence (15) is depicted in Fig. 3.
phase, the superconductivity appears since FC strongly facilitates the superconducting state. In the normal phase, \( T > T_c \), FC causes the linear \( T \) dependence of resistivity, \( \rho(T) \propto T^{19,21,24,32} \), which is in good qualitative agreement with the experimental data on LSCO and La_{2-x}Ce_xCuO_4^{1,20}. We note that in the transition region \( x \gtrsim x_c \) one observes \( \rho(T) \propto T^\alpha \) with \( \alpha \sim 1.0-2.0^{20,21,32} \).

V. CONCLUSIONS

In summary, we have shown that the main physical mechanism, responsible for the unusual properties of the overdoped La_{2-x}Sr_xCuO_4, is the topological quantum phase transition with the emergence of the fermion condensation. This observation can open avenue for chemical preparation of high-\( T_c \) materials with \( T_c \) up to room temperatures. We have concluded our study of exemplifications of the new state of matter reached by fermion condensation with an exploration of high-\( T_c \) superconductors as potential hosts of fermion condensates. In fact, we have shown that the underlying physical mechanism responsible for the unusual properties of the overdoped compound La_{2-x}Sr_xCuO_4 (LSCO) observed recently^{1,2} may very well involve a topological quantum phase transition that induces fermion condensation. Since the topological FC state violates time-reversal symmetry, the Leggett theorem no longer applies. Instead, we have demonstrated explicitly that the superfluid number density \( n_s \) turns out to be small compared to the total number density of electrons. We have also shown that the critical temperature \( T_c \) is a linear function of \( n_s \), while \( n_s(T) \propto T_c - T \). Pairing with such unusual properties is as a shadow of fermion condensation – a situation foretold by an exactly solvable model^{19} long before the experimental observations were obtained by Božović et al.\(^1\) and demonstrating that both the gap and the order parameter exist only in the region occupied by fermion condensate. Thus, the experimental observations\(^1\) can be viewed as a direct experimental manifestation of FC. Additionally, we have demonstrated that at \( T > T_c \) the resistivity \( \rho(T) \) varies linearly with temperature, while for \( x > x_c \) it exhibits metallic behavior, \( \rho(T) \propto T^2 \). Thus, pursuit of a superconductivity formalism adapted to the presence of a fermion condensate captures all the essential physics of overdoped LSCO and successfully explains its most puzzling experimental features, thereby allowing us to close the colossal gap existing between the experiments and Bardeen-Cooper-Schrieffer-like theories. Indeed, these findings are applicable not only to LSCO but also for any overdoped high-temperature superconductor.

FIG. 3: (Color online) The dependence of dimensionless penetration depth \( \lambda/\lambda_0 \) (15) on temperature and doping.
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