Flat bands pinned to the Fermi surface and the phase diagram of electron-doped high-$T_c$ superconductors

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We propose that electron-doped high-$T_c$ compounds possess interaction-induced flat bands pinned to the Fermi surface. This flat-band scenario predicts an enhancement of their critical temperatures $T_c$, relative to BCS theory. In addition to the Fermi-liquid (FL) normal phase, it provides for the existence of two distinct non-Fermi-liquid (NFL) regimes of resistivity, with respective behaviors $ho(T) = ho_0 + A_1 T$ and $ho(T) = ho_0 + A_3/2 T^{3/2}$, with $A_1/T_c$ independent of doping and pressure.

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A central issue confronting present-day condensed matter theory is that of unambiguous determination of the mechanisms governing the rich NFL behavior revealed by intensive experimental studies of strongly correlated electron systems and liquid $^3$He films. Prominent on the scene of this seminal area of condensed matter physics are numerous versions of the Hertz-Millis-Moriya (HMM) approach. These scenarios ascribe such NFL behavior to quantum critical fluctuations, whose impact should be limited to the vicinity of lines of critical temperature $T_c(x)$ or $T_N(x)$ corresponding to observed superfluid or magnetic transitions, where $x$ a relevant control parameter such as doping or magnetic field. However, the experiments in question often furnish clear evidence for the persistence of NFL behavior far from these lines of criticality. Moreover, in liquid $^3$He films where NFL effects are profound, no symmetry inherent in the ground state is broken. It will be argued that it is the single-particle degrees of freedom that are the real playmakers in the observed NFL behavior, rather than critical fluctuations. If so, the traditional mission of integrating them out is futile, akin to throwing the baby out with the bathwater.

Absent any change of symmetry, the posited rearrangement of the Landau state is naturally attributed to some topological transition. In the earliest topological scenario for NFL behavior in homogeneous strongly correlated Fermi systems, advanced more than 20 years ago, this behavior was traced to an interaction-induced rearrangement of the Landau state, often called fermion condensation (FC). This phenomenon, described more vividly as a swelling of the Fermi surface, is associated with the occurrence of a flat band pinned to the Fermi surface. A key signature of a flat band is its topological charge (TC), a topological invariant expressed in terms of a contour integral constructed from the single-particle Green function $G(p,\varepsilon)$ and its derivatives. The TC of a state exhibiting a flat band takes a half-odd-integral value, whereas the TC assigned to a Lifshitz state featuring a multi-connected Fermi surface (or “Lifshitz pockets”) with standard quasiparticle occupation numbers $n(p) = 0, 1$, is always integral.

In a significant formal development, the FC phenomenon was rediscovered in 2009 within the theoretical framework of the adS-CFT duality. More to the point, the formation of flat bands has been demonstrated both analytically and numerically for the Hubbard model, one of the most popular models of strongly correlated electron systems. Therefore the question of principle whether the FC rearrangement exists and is relevant to condensed matter theory already has a positive answer. The remaining issue, addressed herein and elsewhere, is whether or not the FC phenomenon can actually provide the basis for a satisfactory explanation of the experimentally observed behavior of such systems. That the FC scenario competes favorably with other attempts to explain the salient experimental data has been demonstrated in many studies, notably Refs. [11–15]. Additionally, invocation of FC theory has recently resolved a long-standing puzzle associated with the disappearance of a specific set of SdH magnetic oscillations in the 2D electron gas of MOSFETs, which results in the doubling of oscillation periods near a quantum critical point.

The primary goal of this communication is to show how the FC scenario can explain crucial aspects of the phase diagram of the LCCO family of electron-doped high-$T_c$ superconductors, as established empirically in Refs. [2, 3] and reproduced in Fig. 1. We contend that an understanding of the phase diagram of electron-doped high-$T_c$ superconductors, unburdened by the presence of an enigmatic pseudogap phase, is a key step toward unraveling the puzzle of high-$T_c$ superconductivity. A salient feature of the phase diagram presented in Fig. 1 is the presence of two different regimes of NFL temperature variation of the resistivity $\rho(T)$ at $T > T_c$. In the interval $T_c(x) < T < T_1(x)$, the resistivity $\rho(T)$ changes linearly.
with \( T \), thus \( \rho(T) = \rho_0 + A_1 T \), while above \( T_1(x) \) a different NFL regime appears in which \( \rho(T) \) varies as \( T^n \) with \( n \approx 1.6 \).

Since the flat-band scenario has never been applied for electron-doped compounds, a brief presentation of the essential elements of FC theory is in order, focusing on its departures from standard FL theory. The basic equation

\[
\frac{\partial \epsilon(p, T)}{\partial p} = \frac{p}{M} + \int f(p, p') \frac{\partial n(p', T)}{\partial p'} dv',
\]

(1)

of Landau’s FL theory [18] relates the single-particle spectrum \( \epsilon(p) \) (measured from the chemical potential \( \mu \)) to the quasiparticle momentum distribution in terms of a phenomenological interaction function \( f(p, p') \), where \( M \) is the free-fermion mass and \( dv = 2d^3p/(2\pi)^3 \) the three-dimensional volume element. The single-particle energy \( \epsilon(p) \) is connected with the quasiparticle momentum distribution \( n(p) \) via \( n(p, T) = (1 + e^{\epsilon(p, T)/T})^{-1} \), or equivalently by the more convenient expression

\[
\epsilon(p, T) = T \ln \frac{1 - n(p, T)}{n(p, T)}.
\]

(2)

Turning to FC theory, at \( T = 0 \) the basic equation of FC theory takes instead the variational form [5]

\[
\frac{\delta E(n, \lambda)}{\delta n(p)} - \mu = 0, \quad p \in [p_l, p_u],
\]

(3)

with \( \mu \) determined from the Landau postulate that the quasiparticle and particle numbers coincide. Since the left side of this equation is nothing but the quasiparticle energy \( \epsilon(p) \), its solution is indeed found to describe a flat band or fermion condensate on the momentum interval (FC region) \([p_l, p_u]\) having dimensionless width

\[
\eta = (p_u - p_l)/p_F,
\]

within which the quasiparticle occupation number \( n_s(p) \), varies continuously and monotonically from 1 to 0. Outside this FC domain, FL theory still applies, with occupancies \( n_s(p) = 1 \) for \( p < p_l \) and \( n_s(p) = 0 \) for \( p > p_u \).

To facilitate comparison of FC theory with standard FL theory, the basic equation [5] may be recast into a form analogous to that of Eq. (1). This is achieved by differentiation of Eq. (3) with respect to \( p \). Upon adopting the FL relation

\[
\delta \epsilon(p) = \delta \epsilon_0(p) + \int f(p, p') \delta n(p') dv',
\]

(4)

where \( \delta \epsilon_0(p) \) is the variation of the single-particle spectrum of noninteracting quasiparticles (yielding simply \( p/M \) for homogeneous matter), we are then led to equation

\[
0 = \frac{\partial \epsilon_0(p)}{\partial p} + \int f(p, p') \frac{\partial n_s(p', T)}{\partial p'} dv', \quad p, p' \in [p_l, p_u].
\]

(5)

Outside the FC region, the quasiparticle spectrum obeys the Landau-type equation

\[
\frac{\partial \epsilon(p) }{\partial p} = \frac{\partial \epsilon_0(p)}{\partial p} + \int f(p, p') \frac{\partial n_s(p', T)}{\partial p'} dv', \quad p \notin [p_l, p_u].
\]

(6)

The advantage of this reformulation lies in the opportunity to apply the coupled equations [5 and 6] to analysis of the FC phenomenon in electron systems of solids. In so doing, the standard expression \( p/M \) is to be replaced by the corresponding derivative \( \partial \epsilon_0(p)/\partial p \), evaluated, say, within the tight-binding model, or by local-density approximation.

The failure of Eq. (1) in states featuring a flat band is revealed by examining the analytic properties of solutions of this equation in the case where \( f(p, p') \) has no singularities in momentum space. It has been established [15] that its solutions are then necessarily analytic functions of momentum \( p \) in the full momentum space. However, this property is lost if the system hosts a flat band, because the left side of Eq. (3), being the quasiparticle energy, must vanish identically in the FC domain, which cannot occupy the full momentum space. Consequently, the spectrum \( \epsilon(p, n_s) \) of a system exhibiting a FC must be a nonanalytic function of momentum \( p \), for if an analytic function vanishes identically in some domain, it must vanish everywhere. FC solutions \( \epsilon(p, n_s) \) cannot obey Eq. (1). Rather, Eq. (1) must be replaced by the set of two equations [5 and 6], in harmony with the two-component character of the FC phase, containing both the flat band and a complementary system of normal quasiparticles.

Proceeding to finite \( T \), differentiation of Eq. (2) yields

\[
\nu(p) = \frac{\partial \epsilon(p, T)}{\partial p} = -T \frac{\partial n(p, T)/\partial p}{n(p, T)(1 - n(p, T))}.
\]

(7)

Following Nozières [7], one may insert the solution \( n_s(p) \) of Eq. (3) or (6) as a zeroth approximation for \( n_s(p, T) \) that is applicable at low \( T \). The resulting dispersion of the spectrum is then found to be proportional to \( T \) in the FC momentum interval \([p_l, p_u]\). The temperature-dependent generalization of the above FC equations is obtained by inserting Eq. (7) into the right side of Eq. (4) to obtain

\[
-T \frac{n_s(p, T)}{n_s(p, T)(1 - n_s(p, T))} = \frac{p}{M} + \int f(p, p') \frac{\partial n_s(p', T)}{\partial p'} dv'.
\]

(8)

This equation holds in the FC interval \( p \in [p_l, p_u] \), whose width \( \eta \) shrinks with \( T \), vanishing at an upper critical temperature \( T_F \). We now turn to analysis and interpretation of the experimental phase diagram of the 2D LCCO high-\( T_c \) superconductors [2, 3] shown in Fig. 1 where just such an evolution may be traced.

A decisive empirical feature underlying the construction of this diagram is the observed linearity of the re-
that replaces the linear-in-
more, as seen from Fig. 1, it is this second NFL regime
of the two distinct NFL regimes and the coincidence of
The spin-fluctuation scenario fails to explain the presence
ρx(T) = ρ0 + A2T2 with n = 2 for the FL domain (blue),
n = 1 for the NFL domain (red), and n = 1.6 for the
FL Lifshitz-pocket domain (white). The transition line be-
tween the superconducting phase and the antiferromagnetic
or superconducting phases is drawn as a solid curve. The tem-
peratures T1 (triangles) and TFL (inverted triangles), traced
by dashed curves, indicate the crossover temperatures to the
linear-in-T regime of ρ(T) and the FL regimes, respectively.

FIG. 1: (color online) Temperature-doping T − x phase dia-
gram of La2−xCe xCuO4 [2], reprinted with authors’ permis-
sion. The yellow region is the superconducting dome. The resistivity ρ(T) in the different normal phases has the form
ρ(T) = ρ0 + AnTn, with n = 2 for the FL domain (blue),
n = 1 for the NFL domain (red), and n = 1.6 for the
NFL Lifshitz-pocket domain (white). The transition line be-
tween the superconducting phase and the antiferromagnetic
or superconducting phases is drawn as a solid curve. The tem-
peratures T1 (triangles) and TFL (inverted triangles), traced
by dashed curves, indicate the crossover temperatures to the
linear-in-T regime of ρ(T) and the FL regimes, respectively.

sitivity ρ(T) for temperatures above Tc. In the con-
tventional HMM scenarios, this property is attributed to
antiferromagnetic critical fluctuations, which are also as-
sumed to be responsible for the enhancement of the critical
temperature Tc of the superconducting phase transition
[3, 20, 21]. However, in the LCCO family, whose prop-
erties are best studied, there exists an attendant
NFL regime in which ρ(T) ∝ Tn with n ≈ 1.6. This
regime terminates at the same doping xc as the supercon-
ducting phase and the NFL regime in which ρ(T) ∝ T.
The spin-fluctuation scenario fails to explain the presence
of the two distinct NFL regimes and the coincidence of
the critical dopings at which both terminate. Further-
more, as seen from Fig. 1, it is this second NFL regime
that replaces the linear-in-T domain when T is elevated
above 50 K. This additional nonlinear regime is an in-
TEGRAL part of the LCCO phase diagram that cannot plau-
sibly be associated with antiferromagnetic fluctuations
[22].

Fluctuation-induced phenomena such as critical
OPALESCEncence, exhibited as a huge enhancement in absorp-
tion of light by a liquid that is ordinarily transparent,
emerge in the immediate vicinity of points of second-order
phase transitions. The range ∆T of the interval T(N − T
impacted by critical fluctuations on the ordered side of the transition is determined by equating the mean-field value of the order parameter, behaving as √(TN − T), and the corresponding T-independent fluctuation contribution. Accordingly, the stronger the intensity of the fluctua-
tions, the larger the range ∆T, while at |T − TN| > ∆T
any fluctuation scenario fails.

The well-studied heavy-fermion metal YbRh2Si2 [1]
provides the classic example of NFL linear behavior of
ρ(T) in the disordered homogeneous phase, while on the
ordered side of the posited antiferromagnetic phase tran-
sition, T2 resistivity behavior prevails almost up to the
transition temperature TN = 70 mK. The range of the
interval T(N − T) impacted by the critical fluctuations
on the ordered side of the transition is determined by
equating the mean-field value of the order parameter,
behaving as √(TN − T), and the corresponding fluctua-
tion contribution. The observed persistence of FL resis-
tivity ρFL(T) = ρ0 + A2T2 in the ordered phase [1] is
a clear sign of the weakness of the critical fluctuations
and correspondingly small ∆T; otherwise the linear-in-T
corrections to ρFL(T) due to these fluctuations would be
significant. The inescapable conclusion is that the pro-
posed fluctuation mechanism is irrelevant to the NFL
behavior of ρ(T > TN) in this compound.

This example is not alone. Indeed, there are numer-
ous examples of other materials in which the FL law
ρ(T) = ρ0 + A2T2 persists solely on the ordered side
of the transition, while on the disordered side – where,
seemingly, FL theory should be more secure than in the
ordered state – the resistivity varies linearly with T.
Meanwhile, as seen from Fig. 1, as a rule the crossover
from the linear NFL regime ρ(T) ∝ T to the NFL regime
ρ(T) ∝ Tn with n ≈ 1.6 occurs quite far from the lines
of any phase transitions. Furthermore, in the heavy-
fermion metal CeCoIn5, the analogous crossover from the
NFL regime with ρ(T) linear in T to the FL regime with
ρ(T) ∝ T2, occurring as it does in the disordered phase
far from the transition point, is accompanied by a dra-
matic change of the residual resistivity ρ0, which drops
by factor around 10 on the FL side of the crossover [23].
Such a behavior is inconceivable within the textbook un-
derstanding of kinetic phenomena in Fermi liquids. As we
will see, these challenging experimental NFL behaviors
of ρ(T), which defy understanding within a conventional
critical-fluctuation scenario, are amenable to proper ex-
planation if the disordered homogeneous phase contains
a flat band.

Deviations from FL behavior of ρ(T) emerge provided
the overwhelming contributions to the collision integral

I(n) ∝ \int \delta(p1 + p2 − p1′ − p2′)δ(ε1 + ε2 − ε′1 − ε′2) d
v_1′ dv_2′ dv_1 dv_2

(9)

come from regions of momentum space where the Lan-
dau formula ϵ(p) = p_F(p − p_F)/M^*, which assures a T-
independent FL density of states $N(T) \propto 1/v_F \propto M^*$, ceases to hold. Upon changing the integration variable in Eq. (9) from momentum $p$ to energy $\epsilon(p)$, the integrand acquires several factors $dp/d\epsilon(p) = 1/v(p)$. In conventional Fermi liquids these factors are constant. Recalling that the integral itself is proportional to $T^2$, we then arrive at the FL result $\rho(T) = \rho_0 + A_2 T^2$. Now consider instead the flat-band state as described by Eq. (7), and observe that $v(p) \propto 1/T$ holds in the FC momentum interval $[p_1, p_u]$. Accordingly, each momentum integration contributes a factor $\eta/T$ to the collision term and hence to the resistivity. Since $\eta$ is ordinarily very small, we retain only the leading terms of order $\eta$ and $\eta^2$, to arrive at the resistivity

$$\rho_{\text{FC}}(T) = \rho_0(P, x) + A_1(P, x) T,$$  

in the presence of a flat band, with

$$\rho_0(P, x) = \rho_0^* + a_0 \eta^2 P, \quad A_1(P, x) = a_1 \eta P,$$  

wherein $\rho_0^*$ denotes impurity-induced contribution to the residual resistivity $\rho_0$ and $a_0, a_1$ are constants. The total residual resistivity $\rho_0$ becomes dependent on pressure $P$ and doping $x$, facilitating explanation of the unexpected behavior of $\rho_0$ in CeCoIn$_5$ discussed above. (Other observations of such a NFL behavior have also been reported, for example in Ref. [24].)

In Fermi systems with flat bands, still another profound NFL contribution to $\rho(T)$ arises in the momentum region adjacent to the FC domain, where the group velocity $v(p) = dc(p)/dp$ is also suppressed. Its $T$ dependence is readily evaluated in the limit $\eta \to 0$. Straightforward calculations based on Eq. (9), analogous to those performed in Ref. [27], lead to the relation

$$|\epsilon(p \to p_0)| \propto (p - p_0)^2,$$  

which yields a result $v(p) = dc(p)/dp \propto \sqrt{|\epsilon(p)|}$ for the group velocity that holds at small distances outside the FC boundaries $p_l$ and $p_u$ of the flat-band regime. In this case, it is easily verified that the leading contribution to $\rho(T)$ increases as $T^{3/2}$, with the corresponding NFL domain emerging at the same critical doping $x_c$. Thus we infer that four different resistivity regimes come into play in the immediate vicinity of FC onset: (i) the LFL regime $\rho(T) \propto T^2$, (ii) the NFL regime $\rho(T) \propto T^{3/2}$, (iii) the FC regime $\rho(T) \propto T$, and (iv) the high-$T_c$ superconducting regime with $\rho = 0$.

With increasing $T$, the FC interval $\eta$ shrinks to naught at the critical temperature $T_f$. Near $T_f$, the situation is reminiscent of that near the QCP at $T = 0$ as delineated above, with this difference: the relation (12) for the single-particle spectrum $\epsilon(p, T)$ acquires an additional term linear in $T$, and this formula persists for $T > T_f$. As a result, the QCP relation $v(\epsilon) \propto |\epsilon|^{1/2}$ is supplemented by terms linear in $T$. However, at characteristic energies $\epsilon \propto T$, the group velocity $v(\epsilon \simeq T)$ is of order $T^{1/2}$, so that accounting for such a linear-in-$T$ correction to the spectrum makes no difference in the QCP-like behavior $\rho(T) \propto T^{3/2}$ prevailing in the temperature interval $T_1 < T < T_{FL}$. Both limiting temperatures are indicated in Fig. 1.

We are now in position to compare our findings with the experimental phase diagram of the LCCO family reproduced in Fig. 1. As seen, the regimes of $\rho(T)$ that have been identified all meet each other at the critical doping $x_c$. The minor difference between our theoretical predictions and experiment is that in the white NFL regime of Fig. 1, the measured resistivity changes as $T^{1.6}$, while our analysis leads to the relation $\rho(T) = A_3/2 T^{3/2} + A_2 T^2$. This predicted behavior closely resembles the NFL behavior $\rho(T) \propto T^{1.8 \pm 0.1}$ revealed in measurements of the resistivity of the normal state of the heavy-fermion metal CeCoIn$_5$[23], also presumed to host a flat band[13].

Let us now discuss the enhancement of the superconducting critical temperature $T_c$, imputed to critical spin-fluctuations in Refs.[3][21]. Within the competing flat-band scenario, this enhancement may be estimated within the framework of the standard BCS equation

$$1 = V \int \tanh (\epsilon(p, T_c)/2T_c)/2c(p, T_c) dv,$$  

where, for simplicity, the pairing interaction is represented by the constant $V$, ignoring momentum dependence. Performing manipulations based on Eq. (2), this equation takes the form

$$1 = -0.5V[\alpha n / T_c + N_n(0) \ln (\Omega_D/T_c)]$$  

involving the total electron density $n$, the dimensionless FC parameter $\eta$, and a numerical factor $\alpha = O(1)$. In deriving this result, only leading terms divergent at $T_c \to 0$ are retained. The first term in square brackets comes from momentum integration over the FC region. The second, containing the familiar density of states $N_n(0) \propto p_F M^* / \pi^2$, is the usual BCS expression associated with contributions from bands and domains in momentum space where normal quasiparticles reside. In first approximation, the BCS term can be neglected. From Eq. (14) one then finds

$$T_c(x) \propto \eta(x),$$  

i.e., the critical temperature $T_c$ is seen to be a linear function of the FC parameter $\eta$. Comparing Eqs. (15) and (11), we infer that both the $A_1$ term in the resistivity $\rho(T)$ and the critical temperature $T_c$ change with input parameters $P$ and $\eta$ in proportion to the FC parameter $\eta$. Thus, the theoretical ratio $T_c/A_1$ is approximately independent of the input, in agreement with the experimental behavior uncovered in the electron-doped materials LCCO and PCCO, as well as in the Bechgaard class of organic superconductors (TMTSF)$_2$PF$_6$[2,21].
We note in passing that the departure of the effective mass \( M^* \) from the bare mass \( M \), as extracted from experimental data on the specific heat, might be significant, as is the case of heavy-fermion metals. This deviation plays an important role in the magnitude of \( T_c \), as we now demonstrate. First, the effective coupling constant \( V \) in Eq. [13] is eliminated by subtracting from it the BCS relation [13], to obtain

\[
\frac{T_c}{\epsilon_F^0} \ln \left( \frac{T_c}{T_c^{BCS}} \right) = \alpha \frac{M}{M^*} \eta \left( \frac{1}{\eta} \right) \tag{16}
\]

with \( \epsilon_F^0 = p_F^2/2M \). The BCS case \( T_c = T_c^{BCS} \) is realized provided the FC density \( \eta \) goes to zero. Curiously, the BCS situation also applies in heavy-fermion metals, even in the presence of a flat band, owing to the smallness of the ratio \( M/M^* \approx 10^{-2} - 10^{-3} \). This explains why heavy-fermion metals have extremely low \( T_c \) values, a maximum being reached in the heavy-fermion metal CeCoIn5, where does not exceed 2.3 K.

The situation changes when one deals with other electron systems for which \( M/M^* \) is not nearly so small as in heavy-fermion metals. Assuming that the pairing attraction is due to electron-phonon exchange, and choosing \( T_c/M^* = 1, \alpha = 0.1, \) and \( \eta = 0.1 \), one finds

\[
T_c \approx 0.3 \cdot 10^{-2} \epsilon_F^0, \tag{17}
\]

which explains the enhancement of \( T_c \) observed in electron-doped high-\( T_c \) materials. Explication of the enhancement mechanism reflected in this result raises an interesting prospect for the 2D electron gas of MOSFETs and some heterostructures in which attraction in the Cooper channel is furnished by conventional electron-phonon exchange. Beyond a critical density at which a flat band forms and the resistivity becomes linear in \( T \), sufficiently high \( T_c \) values may be reached for a superconducting phase to be detected.

In summary, we have motivated and introduced a set of Landau-like equations that replace the basic equation of Fermi liquid theory connecting the single-particle spectrum and quasiparticle momentum distribution, thereby generalizing the Landau approach to non-Fermi-liquid states possessing a flat band. The results of our analysis of diverse experimental findings demonstrate that the flat-band scenario provides a consistent account of the resistivity as the key kinetic property of superconducting electron-doped materials. Among other seminal results, we have predicted that the critical temperature for a superconducting phase transition in the 2D homogeneous electron gas of MOSFETs may be high enough to be observed in modern experiments. Most significantly, we have demonstrated that the phase diagram of the LCCO family of electron-doped high-\( T_c \) compounds is incisively and economically interpreted within the flat-band scenario developed here. We propose that the successful decoding of such a rich and iconic phase diagram should provide ample incentive for a change of theoretical course in the search for deeper understanding of non-Fermi-liquid phenomena as well as the mechanism of high-\( T_c \) superconductivity.

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