Challenging Magnetic Field Dependence of the Residual Resistivity of the Heavy-Fermion Metal CeCoIn$_5$

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An explanation of paradoxical behavior of the residual resistivity $\rho_0$ of the heavy-fermion metal CeCoIn$_5$ in magnetic fields and under pressure is developed. The source of this behavior is identified as a flattening of the single-particle spectrum, which exerts profound effects on the specific heat, thermal expansion coefficient, and magnetic susceptibility in the normal state, the specific heat jump at the point of superconducting phase transition, and other properties of strongly correlated electron systems in solids. It is shown that application of a magnetic field or pressure to a system possessing a flat band leads to a strong suppression of $\rho_0$. Analysis of its measured thermodynamic and transport properties yields direct evidence for the presence of a flat band in CeCoIn$_5$.

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Measurements of the resistivity $\rho(T)$ in external magnetic fields $H$ have revealed a diversity of low-temperature behaviors of this basic property in heavy-fermion (HF) metals, ranging from the familiar Landau Fermi liquid (LFL) character to challenging non-Fermi liquid (NFL) behaviors. The resistivity $\rho(T)$ is frequently approximated by the formula

$$\rho(T) = \rho_0 + AT^n,$$

where $\rho_0$ is the residual resistivity and $A$ is a $T$-independent coefficient. The index $n$ takes the values 2 and 1, respectively, for FL and NFL behaviors and $1 \leq n \leq 2$ in the crossover between. The term $\rho_0$ is ordinarily attributed to impurity scattering. The application of the weak magnetic field is known to produce a positive classical contribution $\propto H^2$ to $\rho$ arising from orbital motion of carriers induced by the Lorentz force. However, when considering spin-orbit coupling in disordered electron systems where electron motion is diffusive, the magnetoresistivity may have both positive (weak localization) and negative (weak anti-localization) signs.

Our focus here is on the compound CeCoIn$_5$, whose $H-T$ phase diagram is drawn schematically in Fig. 1. Its resistivity $\rho(T, H)$ differs from zero in the region beyond the solid curve that separates the superconducting (SC) and normal states. Above the critical temperature $T_c$ of the SC phase transition, the zero-field resistivity $\rho(T, H = 0)$ varies linearly with $T$. On the other hand, at $T \to 0$ and magnetic fields $H \gtrsim H_2 \approx 5$ T, the curve $\rho(T, H \geq H_2)$ is parabolic in shape. As studied experimentally, CeCoIn$_5$ is one of the purest heavy-fermion metals. Hence the applicable regime of electron motion is ballistic rather than diffusive, and both weak and antiweak localization scenarios are irrelevant. Accordingly, one expects the $H$-dependent correction to $\rho_0$ to be positive and small. Yet this is far from the case: specifically $\rho_0(H = 0) \approx 1.5 \mu\Omega\text{cm}$, while $\rho_0(H = 6 \text{T}) \approx 0.3 \mu\Omega\text{cm}$.

![FIG. 1: (color online). Schematic $T-H$ phase diagram of CeCoIn$_5$. The vertical and horizontal arrows crossing the transition region marked by the thick jagged lines depict the LFL-NFL and NFL-LFL transitions at fixed $H$ and $T$, respectively. As shown by the solid curve, at $H < H_2$ the system is in its superconducting (SC) state, with $H_2$ denoting a quantum critical point hidden beneath the SC dome where the flat band could exist at $H \leq H_\alpha$. The hatched area with the solid curve $T_{\text{crossover}}(H)$ represents the crossover separating the domain of NFL behavior from the LFL domain. A part of the crossover marked with the dots is hidden in the SC state. The NFL state is characterized by the entropy excess $S_\ast$ of Eq. (2).](image)

To resolve this paradox, we suggest that the electron system of CeCoIn$_5$ contains a flat band. Flattening of the single-particle spectrum $\epsilon(p)$ is directly relevant.
to the problem addressed since, due to Umklapp processes, quasiparticles of the flat band produce a contribution to $\rho_0$ indistinguishable from that due to impurity scattering. Furthermore, it is crucial that the flat band somehow becomes depleted at $T \to 0$ and $H = 6$ T, to avoid contradiction of the Nernst theorem. This depletion entails a dramatic suppression of the flat-band contribution to $\rho_0$.

Before proceeding to the analysis of this suppression and its relevance to the behavior observed in CeCoIn$_5$, we call attention to salient aspects and consequences of the flattening of $\epsilon(p)$ in strongly correlated Fermi systems. The theoretical possibility of this phenomenon, also called swelling of the Fermi surface or fermion condensation, was discovered two decades ago (for recent reviews, see[23, 24]). It has received new life in the conceptual framework of topological matter, where it is characterized by nontrivial topology of the Green function in momentum space and associated with topologically protected flat bands[25–27]. At $T = 0$, the ground state of a system having a flat band is degenerate, and therefore the occupation numbers $n_\epsilon(p)$ of single-particle states belonging to the flat band, which form a so-called fermion condensate (FC), are continuous functions of momentum that interpolate between the standard LFL values $(0, 1)$. This leads to an entropy excess

$$S_\epsilon = -\sum_n n_\epsilon(p) \ln n_\epsilon(p) + (1-n_\epsilon(p)) \ln (1-n_\epsilon(p)), \quad (2)$$

which does not contribute to the specific heat $C(T)$. However, in contrast to the corresponding LFL entropy, which vanishes linearly as $T \to 0$, $S_\epsilon$ produces a $T$-independent thermal expansion coefficient $\alpha \propto -\partial S_\epsilon/\partial P^{28, 29}$, where $P$ is the pressure. In its normal state, CeCoIn$_5$ does in fact exhibit a greatly enhanced and almost $T$-independent thermal expansion coefficient[29], so it is reasonable to assert that it possesses a flat band. Analysis of the experimental data on magnetic oscillations[30, 31] supports this assertion. CeCoIn$_5$ is found to have two main Fermi surfaces. The $\alpha$-sheet is observable at all fields down to $H_{c2}$, while the magnetic oscillations associated with the $\beta$-sheet become detectable only at magnetic fields $H \geq 15$ T, behavior in accord with the posited flat character of this band.

In the theory of fermion condensation, the aforementioned ground-state degeneracy is lifted at any finite temperature, where FC acquires a small dispersion proportional to $T$, the spectrum being given by

$$\epsilon(p, n_\epsilon) = T \ln \frac{1-n_\epsilon(p)}{n_\epsilon(p)}. \quad (3)$$

However, the lifting of the degeneracy does not change the FC occupation numbers $n_\epsilon(p)$, implying that the entropy excess $S_\epsilon$ would persist down to zero temperature. To avoid a consequent violation of the Nernst theorem, FC must be completely eliminated at $T \to 0$. In the most natural scenario, this happens by means of a SC phase transition, in which FC is destroyed with the emergence of a pairing gap $\Delta$ in the single-particle spectrum[32, 33].

We propose that this scenario is played out in CeCoIn$_5$ at rather weak magnetic fields $H \ll H_{c2}$, providing for elimination of the flat portion in the spectrum $\epsilon(p)$ and the removal of the entropy excess $S_\epsilon$. In stronger external magnetic fields sufficient to terminate superconductivity in CeCoIn$_5$, this route becomes ineffective, giving way to an alternative scenario involving a crossover from SC state to a state having a multi-connected Fermi surface[34, 35]. In the phase diagram of CeCoIn$_5$ depicted in Fig. 1, such a crossover is indicated by the hatched area between the domains of NFL and LFL behavior and also by the line $T_{cross}(H)$.

We observe that the end point $H_{c0}$ of the curve $T_{cross}(H)$ nominally separating NFL and LFL phases is a magnetic-field-induced quantum critical point (QCP) hidden in the SC state[36]. This is the most salient feature of the phase diagram for the behavior of the resistivity $\rho(T, H)$. Since the entropies of the two phases are different, the SC transition must become first-order near the QCP, in agreement with the experiment[37]. Moreover, LFL behavior remains in effect in the domain $T \to 0$, $H > H_{c2}$. It follows that imposition of fields $H > H_{c2}$ will drive the system from the SC phase to the LFL phase, where FC, or equivalently the flat portion of the spectrum $\epsilon(p)$, is destroyed. Thus, application of a magnetic field $H > H_{c2}$ to CeCoIn$_5$ is predicted to cause a step-like drop in its residual resistivity $\rho_0$, as in fact seen experimentally[38]. Furthermore, it is to be expected that the higher the quality of the CeCoIn$_5$ single crystal, the greater is the suppression of $\rho_0$.

As suggested by this analysis of the $H - T$ phase diagram, the behavior of the dimensionless thermal expansion coefficient, treated as a function of the dimensionless temperature $T_N$, is found to be almost universal. Both the left and right panels of Fig. 2 show that all the normalized data extracted from measurements on CeCoIn$_5$ collapse onto a single scaling curve. As seen from the left panel, the dimensionless coefficient $\alpha_N(T, H) = \alpha(T, H)/\alpha(T_N, H)$, treated as a function of $T_N = T/T_{cross}$, at $T_N < 1$ shows a linear dependence, as depicted by the dash-dot line, implying CeCoIn$_5$ exhibits LFL behavior in this regime. At $T_N \approx 1$ the system enters the narrow crossover region. At $T_N > 1$, NFL behavior prevails, and both $\alpha$ and $S_\epsilon$ cease to depend significantly on $T$, with $\alpha_N$ remaining close to the horizontal line. The observed limiting behaviors, namely LFL with $\alpha \propto T$ and NFL with $\alpha = \text{const.}$, are consistent with recent experimental results[39], as it is seen from the right panel. From this evidence we conclude that essential features of the experimental $T - H$ phase diagram of CeCoIn$_5$ are well represented by Fig. 1.

In calculations of low-temperature transport properties of the normal state of CeCoIn$_5$, we employ a two-band model, one of which is supposed to be flat, with the dispersion given by Eq. 6, while the second band is assumed to possess a LFL single-particle spectrum having...
finite $T$-independent dispersion. We begin the analysis with the case $H = 0$, where the resistivity of CeCoIn$_5$ is a linear function of $T$. As will be seen, this behavior is inherent in electron systems having flat bands. We first express the conductivity $\sigma(T)$ in terms of the imaginary part of the polarization operator $\Pi^{\text{Im}}(j, \omega)$. 

$$\sigma = \lim_{\omega \to 0}^{-1} \text{Im} \Pi(j, \omega) \propto \frac{1}{T} \int \int \frac{dvde}{\cosh^2(\epsilon/2T)} \times |\mathcal{T}(j, \omega = 0)|^2 \text{Im} G_R(p, \epsilon) \text{Im} G_R(p, \epsilon),$$

(4)

where $d\nu$ is an element of momentum space, $\mathcal{T}(j, \omega)$ is the vertex part, $j$ is the electric current, and $G_R(p, \epsilon)$ is the retarded quasiparticle Green function, whose imaginary part is given by

$$\text{Im} G_R(p, \epsilon) = -\frac{\gamma}{(\epsilon - \epsilon(p))^2 + \gamma^2}$$

(5)

in terms of the spectrum $\epsilon(p)$ and damping $\gamma$ referring to the band with the finite value $v_F$ of the Fermi velocity. Invoking gauge invariance, we have $\mathcal{T}(j, \omega = 0) = e\partial \epsilon(p)/\partial p$. Upon inserting this equation into Eq. (4) and performing some algebra we arrive at the standard result

$$\sigma(T) = e^2 n v_F / \gamma(T).$$

(6)

where $n$ is the number density of electrons.

![FIG. 3: Scattering diagrams that contribute to the imaginary part of the mass operator $\Sigma(\epsilon)$, referring to the band with finite value of the Fermi velocity. The single line corresponds to a quasiparticle of that band, and the double line to a FC quasiparticle.](image)

In conventional clean metals obeying LFL theory, the damping $\gamma(T)$ is proportional to $T^2$, leading to Eq. (1) with $n = 2$. NFL behavior of $\sigma(T)$ is due to the NFL temperature dependence of $\gamma(T)$ associated with the presence of FCs. In the standard situation where the volume $\eta$ occupied by FC is rather small, overwhelming contributions to the transport come from inelastic scattering, represented diagrammatically in Fig. 3a and Fig. 3b, where FC quasiparticles (distinguished by the double line) are changed into normal quasiparticles; or vice versa, normal quasiparticles turn into FC quasiparticles. Contributions of these processes to the damping $\gamma$ are estimated on the basis of a simplified formula

$$\gamma(\epsilon) = \eta(\gamma_0 + \gamma_1 \epsilon), \quad \text{Re} \Sigma(\epsilon) = -\eta \gamma_1 \epsilon \ln \frac{\epsilon}{|\epsilon|},$$

(8)

with $\eta$ denoting the volume in momentum space occupied by the flat band, and $\epsilon$ being a characteristic constant, specifying the logarithmic term in $\Sigma$. Accounting for vertex corrections ensures transparent changes in Eq. (7) and cannot be responsible for the effects discussed in our article. We note that Eq. (8) leads to the lifetime $\tau_q$ of quasiparticles, $h/\tau_q \simeq a_1 + a_2 T$, where $h$ is Planck's constant, $a_1$ and $a_2$ are parameters. This result is in excellent agreement with experimental observations. Given this result, one finds that $\rho(T) = \rho_0 + AT$, i.e., the resistivity $\rho(T, H = 0)$ of systems hosting FC is indeed a linear function of $T$, in agreement with experimental data on CeCoIn$_5$. Furthermore, the term $\rho_0$ arises even if the metal has a perfect lattice and no impurities at all.

The presence of the flat band manifests itself not only in kinetics but also in the thermodynamics of CeCoIn$_5$, e.g., in the occurrence of an additional term $\Delta C = C_s -$
\[ C_n \] in the specific heat \( C(T) \), given by

\[ \Delta C = -\frac{1}{2T} \int \left( \frac{d\Delta^2(p)}{dT} \right)_{T_c} n(p)(1 - n(p)) dv, \]

where \( \Delta(p) \) is the energy gap and \( C_s \) and \( C_n \) are the specific heats of superconducting and normal states, respectively. It is FC contribution that endows CeCoIn\(_5\) with a record value of the jump \( \Delta C/C_n = 4.5 \pm 0.3 \) of the specific heat at \( T_c \) (the LFL value being 1.43). The enhancement factor is evaluated by setting \( T = T_c \) in Eq. (9). Importantly, in systems with flat bands, the quantity \( q = -(1/2T_c)(d\Delta^2/dT) \) has the same order\(^\text{as}\) as in LFL theory, where \( q \approx 5 \). To illustrate the point, suppose that the momentum distribution \( n(p) \) depends only on the absolute value of \( p \). One then obtains

\[ \frac{\Delta C(T_c)}{C_n(T_c)} \sim \frac{v_F}{T_c} \int n(p) (1 - n(p)) dp. \]

Thus, the ratio \( \Delta C(T_c)/C_n(T_c) \), shown to be proportional to the volume in momentum space occupied by the flat band, behaves as \( 1/T_c \), implying that \( \Delta C(T_c)/C_n(T_c) \) diverges at \( T_c \to 0 \), in agreement with data on CeCoIn\(_5\), where \( T_c \) is only 2.3 K.

The formula \( \text{Eq. 37} \) can be recast in the form\(^\text{37}\)

\[ \frac{\Delta C(T_c)}{C_n(T_c)} \sim qS^{-1}(T_c) \frac{T_c \chi(T_c)}{C_n(T_c)}, \]

suitable for extracting the Stoner factor \( S(T_c) = \chi(T_c)/\chi_0(T_c) \). Based on the experimental data\(^\text{38}\), one finds \( S(T_c) \sim 0.3 \).

It is straightforward to apply these results to analysis of the slope of the peak of the specific heat in the superconducting state of CeCoIn\(_5\) as \( T \to T_c \), based primarily on Eq. (9). More precisely, one has

\[ \frac{dC(T \to T_c)/dT}{dC_{BCS}(T \to T_c)/dT} = \frac{\Delta C}{C_n(T_c)}, \]

the right side of this relation being evaluated with the aid of Eq. (10). This narrowing of the shape of \( C(T) \) toward the \( \lambda \)-point curve, so familiar in the case of superfluid \(^4\)He, is in agreement with experimental data on CeCoIn\(_5\).

The component of the damping \( \gamma \) linear in energy given by Eq. (8) is responsible for a logarithmic correction to the specific heat \( C(T) \) of the normal state of CeCoIn\(_5\), observed in\(^\text{22}\). With \( f(\varepsilon) = [1 + \varepsilon^2/T]^{-1} \) and \( R(p, \varepsilon) \equiv -\ln(G_R(p, \varepsilon)/G_A(p, \varepsilon)) \), the formula of\(^\text{38}\) for the entropy \( S(T \to 0) \) is recast as

\[ S(T) = -T^{-1} \int dv \int_{-\infty}^{\infty} \varepsilon \frac{df(\varepsilon)}{d\varepsilon} R(p, \varepsilon) d\varepsilon. \]

where, by virtue of Eq. (8), \( R(p, \varepsilon) = \tan^{-1}(\eta/(1 + \eta \ln(|\varepsilon|/|\varepsilon|- \varepsilon(p)/|\varepsilon|)). \) Changing variables to \( w = \varepsilon(p)/\varepsilon \propto (p - p_F)/\varepsilon \) and \( \varepsilon = 2T \) and retaining only leading terms, \( S(T) \) is expressed as the sum \( S = S_+ + S_- \), with

\[ S_\pm \propto T \int_0^\infty \frac{z^2 e^z dz}{(1 + e^z)^2} \int_{-\infty}^{\infty} \tan^{-1} \left[ \frac{\eta}{1 + \eta \ln(\varepsilon/T) \mp w} \right] dw. \]

\[ \text{Eq. 14} \]

These integrals are evaluated analytically to yield \( S(T) = S_{FL}(T) \sim \eta T \ln T \), in agreement with available experimental data on the specific heat of CeCoIn\(_5\).

Now we show that the application of field \( H > H_{c2} \) on CeCoIn\(_5\) generates the step-like drop in the residual resistivity \( \rho_0 \). Indeed, as seen from Fig. 1 at low temperatures \( T < T_{cross} \), the application of fields \( H > H_{c2} \) drives the system from the SC state to the LFL one, where the flat portion of \( \varepsilon(p) \) is destroyed. Thus, the term \( \eta \) vanishes strongly reducing \( \rho_0 \). The suppression of \( \rho_0 \) in magnetic fields is associated with another NFL phenomenon recently observed in CeCoIn\(_5\). This is the deviation of the temperature dependence of the amplitude of magnetic oscillations \( A(T) \) from the standard Lifshitz-Kosevich-Dingle form

\[ A(T) = A_D (X/\sinh X). \]

\[ \text{Eq. 15} \]

Here \( A_D \propto e^{-Y} \) is the Dingle factor, while \( Y = 2\pi^2 k_B T_D/\omega_c \), \( X = 2\pi^2 k_B T/\omega_c \), \( T_D \) is the Dingle temperature, and \( \omega_c \) is the cyclotron frequency. Conventionally \( T_D \), assumed to be constant, is associated with impurity scattering. More generally, \( T_D \) is related to the value of \( \rho_0 \) in Eq. (1), which, as we have seen, becomes \( T-dependent \) in a system with a flat band. Why? Because the flat band, in the present context, guarantees an overwhelming contribution to \( \rho_0 \) that must disappear at \( T < T_{cross} \) to evade violation of the Nernst theorem. This inexorable sequence triggers the abrupt downward jump of \( \rho_0 \) and of \( T_{D} \) correspondingly, leading in turn to an upward jump of the Dingle factor \( A_D \) near \( T_{cross} \), which agrees with observations\(^\text{22}\). In parallel with this challenging behavior of the residual resistivity in magnetic fields, it is appropriate to address the behavior of \( \rho_0 \) versus pressure \( P \), studied in CeCoIn\(_5\) experimentally in\(^\text{22}\). At \( P > P^* = 16 \text{ GPa} \), \( \rho_0 \) drops reversibly by one order of magnitude to a very small value of about 0.2 \( \mu \Omega \text{cm} \). We can reasonably infer that the application of pressure eliminates FC\(^\text{129}\), triggering a jump in \( \rho_0 \) to the lower value measured. It should be emphasized that a nonzero contribution of FC to \( \rho_0 \) is associated with the presence of the crystal lattice, more precisely, with the Umklapp processes, violating momentum conservation. At the same time, such a restriction is absent in dealing with the thermal resistivity \( \omega_0 \). If, as usual, one normalizes the thermal resistivity by \( w = \pi^2 k_B^2 / (3e^2 \kappa) \) where \( \kappa \) is the thermal conductivity, the famous Wiedemann-Franz relation then reads \( \rho_0 = \omega_0 \). The distinguished role of the Umklapp processes in the occurrence of \( \rho_0 \) in Fermi systems with FC implies that in the presence of FC, the Wiedemann-Franz law is violated so that \( \rho_0 < \omega_0 \). In CeCoIn\(_5\) this violation does take the place\(^\text{22}\).
In summary, we have shown that the application of magnetic fields and pressure on CeCoIn5 leads to strong suppression of the residual resistivity $\rho_0$. By considering the behavior of the thermal expansion coefficient, the specific heat, and the amplitude of magnetic oscillations, we have unveiled the roles played by the flat band in thermodynamic as well as in transport properties of CeCoIn5. Our considerations furnish strong evidence for the presence of flat band in CeCoIn5, which thereby becomes the member of a long-expected class of Fermi liquids.

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