Phase Diagram of Heavy Fermion Metal CeCoIn$_5$

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We present a comprehensive analysis of the low temperature experimental $H - T$ phase diagram of CeCoIn$_5$. The main universal features of the diagram can be explained within the Fermi-liquid theory provided that quasiparticles form so-called fermion-condensate state. We show that in this case the fluctuations accompanying an ordinary quantum critical point are strongly suppressed and cannot destroy the quasiparticles. Analyzing the phase diagram and giving predictions, we demonstrate that the electronic system of CeCoIn$_5$ provides a unique opportunity to study the relationship between quasiparticles properties and non-Fermi liquid behavior.

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Although much theoretical efforts have been spared to understand the non-Fermi liquid behavior (NFL) of heavy fermion (HF) metals using the concept of quantum critical points, the problem is still far from its complete understanding since the experimental systems display serious discrepancies with the theoretical predictions [1]. Common belief is that a quantum critical point (QCP) is the point where a second order phase transition occurs at temperature $T \to 0$, and where both thermal and quantum fluctuations are present destroying quasiparticles and generating a new regime around the point of instability between two stable phases. Recent experimental studies of the CeCoIn$_5$ HF metal provide valuable information about the NFL behavior near possible QCP due to its excellent tunability by a pressure $P$ and/or a magnetic field $H [2, 3, 4]$. The experimental studies have shown that besides a complicated $H - T$ phase diagram, the normal and superconducting properties around the QCP exhibit various anomalies. One of them is power (in both $T$ and $H$) variation of the resistivity and heat transport [2, 5, 6, 7, 8], inherent to both NFL and Landau Fermi liquid (LFL) regimes. The other one is a continuous magnetic field evolution of a superconductive phase transition from the second order to the first one [9, 10]. Above anomalous power laws can be hardly accounted for within scenarios based on the QCP occurrence with quantum and thermal fluctuations. For example, the divergence of the normal-state thermal expansion coefficient, $\alpha/T$ is stronger than that in the 3D itinerant spin-density-wave (SDW) theory, but weaker than that in the 2D SDW picture [11]. This brings the question of whether the fluctuations are responsible for the observed behavior, and if they are not, what kind of physics determines the above anomalies? On the other hand, the direct observations of quasiparticle band in CeIrIn$_5$ have been reported recently [12]. However, if the quasiparticles do exist, why they are not suppressed by the fluctuations?

In this letter we show that these problems can be resolved within LFL theory provided that quasiparticles form the so-called fermion-condensate (FC) state emerging behind the fermion condensation quantum phase transition (FCQPT) [13]. We show that near FCQPT the fluctuations are strongly suppressed while FC by itself is "protected" from above fluctuations by the first order phase transition. We analyze the experimental $H - T$ phase diagram of CeCoIn$_5$ and show that its main universal features can be well understood within the theory based on FCQPT. We demonstrate that the electronic system of CeCoIn$_5$ can be shifted from the ordered to disordered side of FCQPT by a magnetic field, therefore giving a unique possibility to study the relationship between quasiparticles and NFL behavior.

To study the low temperature universal features of HF metals, we use the notion of HF liquid in order to avoid the complications related to the crystalline anisotropy of solids. This is possible since we consider the (universal) behavior related to the power-law divergences of observables like the effective mass, thermal expansion coefficient etc. These divergences are determined by small (as compared to those from unit cell of a corresponding reciprocal lattice) momenta transfer so that the contribution from larger momenta can be safely ignored.

Let us consider HF liquid characterized by the effective mass $M^*$. Upon applying the well-known equation, we can relate $M^*$ to the bare electron mass $M$ [17]

$$M^* = \frac{1}{1 - N_0 F^1(p_F, p_F)/3}$$

(1)

Here $N_0$ is the density of states of a free electron gas, $p_F$ is Fermi momentum, and $F^1(p_F, p_F)$ is the $p$-wave component of Landau interaction amplitude. Since LFL theory implies the quasiparticle density in the form $x = p_F^3/3\pi^2$, we can rewrite the amplitude as $F^1(p_F, p_F) = F^1(x)$. When at some $x = x_{FC}$, the $F^1(x)$ achieves some critical value, the denominator in Eq. (1) tends to zero so that the effective mass diverges at $T = 0$. Beyond the critical point $x_{FC}$ the denominator becomes negative making the effective mass negative. To avoid physically meaningless states with $M^* < 0$, the system undergoes
FCQPT with FC formation in the critical point \( x = x_{\text{FC}} \). Therefore, behind the critical point \( x_{\text{FC}} \) the quasiparticle spectrum is flat, \( \varepsilon(p) = \mu \), in some region \( p_i \leq p \leq p_f \) of momenta, while the corresponding occupation number \( n_0(p) \) varies continuously from 1 to 0, \( 0 < n_0(p) < 1 \). Here \( \mu \) is a chemical potential.

To investigate the FC state at \( T = 0 \), we apply weak BCS-like interaction \[18\] with the coupling constant \( \lambda \) and see what happens with the superconducting order parameter \( \kappa(p) \) as \( \lambda \to 0 \). To do so, we express \( \kappa(p) \) via the frequency integral from Gorkov function \( F^+ \). To find latter function, we use the usual pair of equations for functions \( F^+ \) and \( G \) (see e.g. Ref. \([16]\)). The solution of above equations yields

\[
F^+(k, \omega) = i \lambda < \kappa(p) > \frac{1}{2 \pi E_1(p)} \left[ \frac{1}{\omega - E_1(p) + i0} - \frac{1}{\omega + E_1(p) - i0} \right],
\]

\[
G(k, \omega) = \frac{1 - n(p)}{\omega - E_1(p) + i0} + \frac{n(p)}{\omega + E_1(p) - i0},
\]

where the superconducting gap,

\[
\Delta(p) = -\lambda < \kappa(p) >= -\lambda \int \kappa(p) \frac{d^3k}{(2\pi)^3},
\]

with

\[
\kappa(p) = \int_{-\infty}^{\infty} F^+(p, \omega) \frac{d\omega}{2\pi},
\]

is related to the dispersion \( \varepsilon(p) \) as

\[
\varepsilon(p) - \mu = \Delta(p) \frac{1 - 2v^2(p)}{2\kappa(p)}.
\]

Here \( n(p) = v^2(p) \), the superconducting order parameter \( \kappa(p) = u(p)v(p) = \sqrt{n(p)(1-n(p))} \), \( u(p) \) and \( v(p) \) are the coefficients of corresponding Bogoliubov transformation, \( u^2(p) + v^2(p) = 1 \). Next we observe from Eqs. (3) and (5) that when \( \lambda \to 0 \) the dispersion \( \varepsilon(p) \) becomes flat, while Eq. (2) in the lowest order in \( \lambda \) becomes

\[
F_0^+(k, \omega) = -i \sqrt{n_0(p)(1-n_0(p))} \left[ \frac{1}{\omega + i0} - \frac{1}{\omega - i0} \right],
\]

\[
G_0(k, \omega) = \frac{1 - n_0(p)}{\omega + i0} + \frac{n_0(p)}{\omega - i0},
\]

\[
\varepsilon(p) - \mu = 0.
\]

To check this answer, we integrate \( F_0^+ \) over frequencies,

\[
\int_{-\infty}^{\infty} F_0^+(p, \omega) \frac{d\omega}{2\pi} = \sqrt{n_0(p)(1-n_0(p))},
\]

and conclude that \( \kappa(p) = \sqrt{n_0(p)(1-n_0(p))} \).

Since in our model the transition temperature \( T_c \sim \Delta \sim \lambda \to 0 \), the order parameter \( \kappa(p) \) vanishes at any finite temperature so that the quasiparticle occupation number is given by Fermi-Dirac function which we represent in the form

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

Observing that at \( T \to 0 \) the distribution function satisfies the inequality \( 0 < n_0(p, T) < 1 \) at \( p_i \leq p \leq p_f \), we conclude that both the entropy \( S \) and the logarithm in the right hand side of Eq. (3) are finite even at \( T \to 0 \). In this case, the entropy \( S_{\text{NFL}} \) is related to the special solution \( n_0(p) \) and contains the temperature independent term \( S_0 = S_{\text{NFL}}(T \to 0) \). For this special solution \( n_0(p) \) the dispersion is flat, \( \varepsilon(p) = \mu \) \[20\]. Thus, the occupation number \( n_0(p) \) represents the special solutions of both BCS and LFL equations determining the NFL behavior of HF liquid. Namely, as it follows from Eq. (7), contrary to conventional BSC case, the FC solutions are characterized by infinitesimal value of superconducting gap, \( \Delta \to 0 \), while the order parameter \( \kappa_0(p) \) remains finite and the entropy \( S = 0 \). At the same time, in contrast to the standard solutions of the LFL theory, the special ones are characterized by the finite superconducting order parameter \( \kappa(p) \) at \( T = 0 \). At \( T \to 0 \) both the normal state of the HF liquid with the finite entropy \( S_{\text{NFL}} \) and the BCS state with \( S = 0 \) coexist being separated by the first order phase transition where the entropy undergoes a finite jump \( \delta S = S_0 \). Due to 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, both at the FCQPT point and behind it there are no critical fluctuations accompanying second order phase transitions and suppressing the quasiparticles. As a result, the quasiparticles survive and define the thermodynamic properties of the HF system.

On the basis of above special solutions peculiarities we can explain the main universal properties of the \( H - T \) phase diagram of the HF metal CeCoIn\(_5\) shown in Fig. 1. The latter substance is a superconductor with \( T_c = 2.3 \) K, while a field tuned QCP with a critical field of
$H_{c2} = 5.1$ T coincides with $H_{c1}$, the upper critical field where superconductivity vanishes \([1, 2]\). We note that in some cases $H_{c1} = 0$. For example, CeRu$_2$Si$_2$ shows no magnetic ordering down to lowest temperatures \([21]\). Therefore, in our simple HF model $H_{c2}$ can be treated as fitting parameter. It follows from the above consideration that $H_{c1} \simeq H_{c2}$ is an accidental coincidence. Indeed, $H_{c1}$ is determined by $\lambda$ which, in turn, is given by the coupling of electrons with magnetic, phonon, etc. excitations rather than by $H_{c2}$. As a result, under application of a pressure which influences differently $\lambda$ and $H_{c1}$, the above coincidence will be removed. This is in agreement with the facts from Ref. \([3]\).

At relatively high temperatures, the superconducting-normal phase transition in CeCoIn$_5$ shown by the solid line in Fig. 1 is of the second order \([3, 10]\). In that case, the entropy and the other thermodynamic quantities are continuous at the transition temperature $T_c(H)$. Since $H_{c1} \simeq H_{c2}$, upon the application of magnetic field, the HF metal transits to its NFL state down to lowest temperatures as seen from Fig. 1. As long as the phase transition is of the second order, the entropy of SC phase $S_{SC}(T)$ coincides with the entropy $S_{NFL}(T)$ of NFL state, 

$$S_{SC}(T \to T_c(H)) = S_{NFL}(T \to T_c(H)). \quad (10)$$

Since $S_{SC}(T \to 0) \to 0$, Eq. \([10]\) cannot be satisfied at sufficiently low temperatures due to the presence of temperature-independent term $S_0$. Thus, in accordance with experimental results \([9, 10]\), the second order phase transition converts to first order one below some temperature $T_0(H)$. The prediction that the superconducting phase transition may change its order had been made in the early 1960’s \([19]\). This prediction is corroborated by our general analysis based on Eq. \([110]\). Namely, if the superconducting phase were replaced by some other ordered phase separated from the NFL phase by the second order phase transition at $H = 0$, then at some temperature $T_0(H)$ this phase transition should change its order. In our case the NFL phase plays a role of disordered one. But, as it follows from above consideration, the NFL phase has the temperature independent entropy term $S_0$. Since in the ordered phase the Nernst theorem ($S \rightarrow 0$ as $T \rightarrow 0$) should hold, we come to conclusion that there is the entropy step (from $S_0$ to zero) as $T \rightarrow 0$ while a system traverses the phase transition line from ordered phase to NFL one. This means that this phase transition should change its order at $T_0(H)$. For example, the AFM phase transition with $T_{N}(H)$ (representing the field dependence of Néel temperature) should become first order at some finite temperature $T_0(H)$. Besides the jump in the entropy, this first order transition, for example, should result in a jump in the sample length, corresponding to a divergence of $\alpha = -\partial S/\partial P$. Under constant entropy (adiabatic) conditions, there should be a temperature step as a magnetic field crosses the above phase boundary due to inequality \([9]\). Indeed, the entropy jump would release the heat, but since $S = const$ the heat is absorbed, causing the temperature to decrease in order to keep the constant entropy of the NFL state. Note that the minimal jump is given by the temperature-independent term $S_0$, which can be quite large so that the corresponding HF metal can be used as an effective cooler at low temperatures.

The entropy $S_{NFL}$ determines the anomalous behavior of CeCoIn$_5$ in the NFL region of the phase diagram. The term $S_0 \sim (p_f - p_i)/p_F$ can be determined from the experimental data on spin susceptibility (following Curie law) and the specific heat jump $\Delta C$ at $T_c$ \([23]\). In HF metals like CeCoIn$_5$ the normalized jump $\Delta C/C_n \approx 4.5$ is substantially higher than the ordinary BCS value \([23]\), where $C_n$ is the specific heat of a normal state. In the case of FC, the specific heat jump is not proportional to $T_c$ and is related to the fermion condensate parameter $\delta_{FC} = (p_f - p_i)/p_F$, therefore the normalized jump $\Delta C/C_n$ can be large \([24, 25]\). This estimation gives $\delta_{FC} \approx 0.044$ \([25]\). The entropy $S_{NFL}$ determines also both thermal expansion coefficient $\alpha = -\partial S/\partial P$ and Gruneisen ratio $\Gamma = \alpha/C_n$ of Fermi liquids with FC \([20, 22, 23]\). Since the entropy has the temperature independent part $S_0$, the thermal expansion coefficient $\alpha \simeq -\partial S_0/\partial P$ becomes temperature independent at low temperatures. Therefore, at $T \to 0 \alpha(T) \to const$ while the specific heat $C_n(T) \to 0$. As a result, $\Gamma(T \to 0)$ diverges in coincidence with the facts from Ref. \([11]\).
Now we consider the LFL behavior tuned by a magnetic field $H \geq H_d$. Since the NFL behavior of CeCoIn$_5$ coincides with that of YbRh$_2$(Si$_{0.53}$Ge$_{0.47}$)$_2$ and YbRh$_2$Si$_2$ [24, 27] we would expect that the LFL behavior of these substances would also coincide. For example, in YbRh$_2$(Si$_{0.53}$Ge$_{0.47}$)$_2$ the scattering coefficient $A(H)$ in the resistivity $\rho = \rho_0 + AT^2$, with $\rho_0$ being the temperature independent part, diverges as $A(H) \propto (H - H_d)^{-1}$ [20] while in CeCoIn$_5$ it diverges as $A(H) \propto (H - H_d)^4$ with the exponent $c \approx -4/3$ [8, 13]. In magnetic fields, the exponent $c = -1$ characterizes the function $A(H)$ of HF liquid with FC [28], while the exponent $c = -4/3$ describes the function $A(H)$ of HF liquid on the disordered side of FC [28, 29].

To understand this striking change in the behavior of CeCoIn$_5$, we recall that FC has just appeared in this substance since $\delta p_{FC} = (p_f - p_1)/p_F \simeq 0.044 \ll 1$. As soon as magnetic field is sufficiently high, $H \geq H_{cr}$ ($H_{cr}$ is a critical field destroying FC state), Zeeman splitting $\delta p_F = (p_{F1} - p_{F2})/p_F$ of the two Fermi surfaces of HF liquid exceeds the condensate parameter, $\delta p_F \simeq p_{FC}$, and the HF liquid with FC becomes LFL placed on the disordered side near QCP. Here $p_{F1}$ and $p_{F2}$ are the Fermi momenta of the two Fermi surfaces formed by the application of a magnetic field. The splitting can be estimated as $p_F^2 \delta p_F/(M^*(H)) \sim H \mu_B$, where $\mu_B$ is Bohr magneton. Taking into account that $A(H) \propto (M^*(H))^2$ we obtain $(H_{cr} - H_d)/H_d \sim (c_1 \delta p_F)^3$. Our estimations of the coefficient $c_1$ based on the experimental function $A(H)$ show that $c_1 \sim 5$, and we obtain that reduced field $(H_{cr} - H_d)/H_d \sim (c_1 \delta p_F)^3 \approx 0.02$. Thus, we can safely suggest that the reduced field of 0.02 is much smaller than minimal reduced field 0.1 where $A(H)$ measurements have been carried out in Ref. [4, 11]. As a result, the electronic system of CeCoIn$_5$ is placed on the disordered side of FCQPT by the application of such high field and reveals $A(H) \propto (H - H_d)^{-4/3}$. We can see from the inset to Fig.1 that the coefficient $B(H)$ has the same critical field dependence. Here $B(H)$ stands for the $T^2$-dependent contribution to the thermal resistivity and related to $A(H)$ by a field-independent factor, $A(H)/B(H) \approx 0.47$, as it should be in the case of ordinary metals [4]. We conclude that the LFL behavior of CeCoIn$_5$ corresponds to the LFL behavior of HF liquid placed on the disordered side of FCQPT [31]. At decreasing field when $H < H_{cr}$, we predict that the exponent $c$ will change from $c = -4/3$ to $c = -1$.

At finite temperatures, the system remains in the LFL state, but there exists a temperature $T^*(H)$ where the influence of FC is recovered and the related NFL behavior is restored. To calculate the function $T^*(H)$, we observe that the effective mass $M^*$ cannot be changed at $T^*(H)$. Since at $T > T^*(H)$ the effective mass $M^*(T) \propto 1/T$ [30] at $T < T^*(H)$, $M^*(H) \propto (H - H_d)^{-2/3}$, we have $T^*(H) \propto (H - H_d)^{-2/3}$. In high magnetic fields, there is a new crossover line because the effective mass starts to depend on temperature as $M^*(T) \propto T^{-2/3}$ [29, 31] and $T^*(H)$ becomes $T^*(H) \propto (H - H_d)$. As it is seen from Fig. 1, the obtained results are in good agreement with experimental facts. It is worth to note that the recovery of FC state can be observed in measurements of a tunneling conductivity which is expected to be noticeably asymmetrical with respect to the change of voltage bias from $V$ to $-V$ in Fermi systems with FC [32]. This asymmetry can be observed when the HF metal with FC is either normal or superconducting because the asymmetry is indeed determined by the violation of the so-called particle-hole symmetry, while this symmetry holds within the LFL theory. This asymmetry is not supported by FC occupation number $n_0(p, T)$ since it does not evolve from the Fermi-Dirac distribution function. Therefore, the tunneling conductivity is asymmetrical when HF metal is superconducting, it does not change at $T = T_c$ and gradually vanishes at rising temperatures. We note also that such behavior of the conductivity has recently been observed experimentally in CeCoIn$_5$ [33]. On the other hand, the behavior of the conductivity can be different when the HF metal transits from its LFL to NFL states. We predict that in the case of CeCoIn$_5$ the conductivity being symmetrical in the LFL regime becomes gradually asymmetrical reaching its maximum in the NFL state at elevated temperatures when $T > T^*(H)$ and eventually vanishes.

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