Behavior of the antiferromagnetic phase transition near the fermion condensation quantum phase transition in YbRh$_2$Si$_2$

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1. Introduction

Fundamental understanding of the low-temperature physical properties of such strongly correlated Fermi systems as heavy fermion (HF) metals in the vicinity of a quantum phase transition persists as one of the most challenging objectives of condensed-matter physics. List of these extraordinary properties are markedly large. Recent exciting measurements on YbRh$_2$Si$_2$ at the second order antiferromagnetic (AF) phase transition extended the list and revealed a sharp peak in low-temperature specific heat, which is characterized by the critical exponent $\alpha \approx 0.38$ and therefore differs drastically from those of the conventional fluctuation theory of second order phase transitions [1], where $\alpha \approx 0.1$ [2]. The obtained large value of $\alpha$ casts doubts on the applicability of the conventional theory and sends a real challenge for theories describing the second order phase transitions in HF metals [1], ignoring strong theoretical effort to explain the violation of the critical universality in terms of the tricritical point [3–6].

The striking feature of the fermion condensation quantum phase transition (FCQPT) is that it has profound influence on thermodynamically driven second order phase transitions provided that these take place in the non-Fermi liquid (NFL) region formed by FCQPT [7,8]. As a result, the curve of any second order phase transition passes into a curve of the first order one at the tricritical point leading to a violation of the critical universality of the fluctuation theory. For example, the second order superconducting phase transition in CeCoIn$_5$ changes to the first one in the NFL region [9]. As we shall see, it is this feature that gives the key to resolve the challenge.

It is a common wisdom that low-temperature and quantum fluctuations at quantum phase transitions form the specific heat, magnetization, magnetoresistance, etc., which are drastically different from that of conventional metals [10–14]. Usual arguments that quasiparticles in strongly correlated Fermi liquids “get heavy and die” at a quantum critical point commonly employ the well-known formula basing on assumptions that the $z$-factor (the quasi-particle weight in the single-particle state) vanishes at the points of second order phase transitions [15]. However, it has been shown that this scenario is problematic [16]. On the other hand, facts collected on HF metals demonstrate that the effective mass strongly depends on temperature $T$, doping (or the number density) $x$, ap-
plied magnetic fields $B$, etc., while the effective mass $M^*$ itself can reach very high values or even diverge, see e.g. [12,13]. Such a behavior is so unusual that the traditional Landau quasiparticles paradigm does not apply to it. The paradigm says that elementary excitations determine the physics at low temperatures. These behave as Fermi quasiparticles and have a certain effective mass $M^*$ which is independent of $T$, $x$, and $B$ and is a parameter of the theory [17]. A concept of FCQPT preserving quasiparticles and intimately related to the unlimited growth of $M^*$ had been developed in Refs. [7,18,19]. In contrast to the Landau paradigm based on the assumption that $M^*$ is a constant, the FCQPT approach supports an extended paradigm, the main point of which is that the well-defined quasiparticles determine the thermodynamic and transport properties of strongly correlated Fermi systems, $M^*$ becomes a function of $T$, $x$, $B$, while the dependence of the effective mass on $T$, $x$, $B$ gives rise to the non-Fermi liquid behavior [8,20–23]. Studies show that the extended paradigm is capable to deliver an adequate theoretical explanation of the NFL behavior in different HF metals and HF systems [8,9,20,22–25].

In the present short communication, we analyze the specific-heat measurements on YbRh$_2$Si$_2$ in the vicinity of the second order AF phase transition with $T_{N1} = 72$ mK [1]. The measurements reveal that the corresponding critical exponent $\alpha = 0.38$ which differs drastically from that produced by the fluctuation theory of second order phase transitions, where $\alpha \approx 0.1$. We show that under the application of magnetic field $B$ the curve $T_{N2}(B)$ of the second order AF phase transitions in YbRh$_2$Si$_2$ passes into a curve of the first order ones at the tricritical point with temperature $T_{cT} = T_{N2}(B_{cT})$. This change is generated by FCQPT. Near the tricritical point the Landau theory of second order phase transitions is applicable and gives $\alpha \approx 1/2$ [2]. This value of $\alpha$ is in good agreement with the specific-heat measurements describing the data in the entire temperature range around the AF phase transition. As a result, we conclude that the critical universality of the fluctuation theory is violated at the line of the AF phase transitions due to the tricritical point.

2. Fermion condensation quantum phase transition

We start with visualizing the main properties of FCQPT. To this end, consider the density functional theory for superconductors (SCDFT) [26]. SCDFT states that the thermodynamic potential $\Phi$ is a universal functional of the number density $n(r)$ and the anomalous density (or the order parameter) $\kappa(r, r_1)$ and provides a variational principle to determine the densities [26]. At the superconducting transition temperature $T_c$, a superconducting state undergoes the second order phase transition. Our goal now is to construct a quantum phase transition which evolves from the superconducting one.

Let us assume that the coupling constant $\lambda$ of the BCS-like pairing interaction vanishes, $\lambda \to 0$, making vanish the superconducting gap at any finite temperature. In that case, $T_c \to 0$ and the superconducting state takes place at $T = 0$ while at finite temperatures there is a normal state. This means that at $T = 0$ the anomalous density

$$\kappa(r, r_1) = \langle \Psi^\dagger(r) \Psi(r_1) \rangle$$

is finite, while the superconducting gap

$$\Delta(r) = \lambda \int \kappa(r, r_1) \, dr_1$$

is infinitely small [8,9]. In Eq. (1), the field operator $\Psi_\sigma(r)$ annihilates an electron of spin $\sigma$, $\sigma = \uparrow, \downarrow$ at the position $r$. For the sake of simplicity, we consider a homogeneous electron liquid [8]. Then at $T = 0$, the thermodynamic potential $\Phi$ reduces to the ground state energy $E$ which turns out to be a functional of the occupation number $n(p)$ since the order parameter $\kappa(p) = \sqrt{n(p)(1-n(p))}$ [23,26–28]. Upon minimizing $E$ with respect to $n(p)$, we obtain [8,18]

$$\left. \frac{\delta E}{\delta n(p)} \right|_{n(p)} = \varepsilon(p) = \mu,$$

(3)

where $\mu$ is the chemical potential. As soon as Eq. (3) has nontrivial solution $n_0(p)$ then instead of the Fermi step, we have $0 < n_0(p) < 1$ in certain range of momenta $p_i < p < p_f$ with $\varepsilon(p) = \sqrt{\rho_0(p)(1 - \rho_0(p))}$ is finite in this range, while the single-particle spectrum $\varepsilon(p)$ is flat. Thus, the step-like Fermi filling inevitably undergoes restructuring and forms the fermion condensate (FC) when Eq. (3) possesses for the first time the nontrivial solution at some quantum critical point (QCP) $x = x_c$. Here $p_F$ is the Fermi momentum and $x = p_F^3/3\pi^2$. In that case, the range vanishes, $p_1 \to p_f \to p_i$, and the effective mass $M^*$ diverges at QCP [8,18,20,22]

$$\frac{1}{M^*(x-x_c)} = \frac{1}{p_F} \frac{\partial \varepsilon(p)}{\partial p} \bigg|_{p=p_F, x-x_c} \to 0.$$

(4)

At any small but finite temperature the anomalous density $\kappa$ (or the order parameter) decays and, as we shall see, this state undergoes the first order phase transition and converts into a normal state characterized by the thermodynamic potential $\Phi_0$. At $T = 0$, the entropy $S = -\mu \Phi_0/\partial T$ of the normal state is given by the well-known relation [17]

$$S_0[n_0(p)] = -2 \int [n_0(p) \ln(n_0(p)) + (1 - n_0(p)) \ln(1 - n_0(p))] \frac{dp}{(2\pi)^3},$$

(5)

which follows from combinatorial reasoning. It is seen from Eq. (5) that the normal state is characterized by the temperature-independent entropy $S_0$ [8,27]. Since the entropy of the superconducting ground state is zero, we conclude that the entropy is discontinuous at the phase transition point, with its discontinuity $\Delta S = S_0$. Thus, the system undergoes the first order phase transition. The heat $q$ of transition from the asymmetrical to the symmetrical phase is $q = T_c S_0 = 0$ because of the stability condition at the point of the first order phase transition, we have $\Phi_0(n(p)) = \Phi(\kappa(p))$. Obviously the condition is satisfied since $q = 0$. At $T = 0$, a quantum phase transition is driven by a nonthermal control parameter, e.g. the number density $x$. To clarify the role of $x$, consider the effective mass $M^*$ which is related to the bare electron mass $M$ by the well-known Landau equation [17]

$$\frac{1}{M^*} = \frac{1}{M} + \int \frac{p_f p_1}{p_f^3} F(p_f, p_1) \frac{\partial n(p, T)}{\partial p_1} \frac{dp_1}{(2\pi)^3}.$$

(6)

Here we omit the spin indices for simplicity, $n(p, T)$ is quasiparticle occupation number, and $F$ is the Landau amplitude. At $T = 0$, Eq. (6) reads [29,30]

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

(7)

Here $N_0$ is the density of states of a free electron gas and $F^3(\chi)$ is the $p$-wave component of Landau interaction amplitude. When at some critical point $x = x_c$, $F^3(\chi)$ achieves certain threshold value, the denominator in Eq. (7) tends to zero so that the effective mass diverges at $T = 0$ [29,30]. It follows from Eq. (7) that beyond the critical quantum point $x_c$, the effective mass becomes negative. To avoid unstable and physically meaningless state with a negative effective mass and in accordance with Eq. (4), the system must undergo a quantum phase transition at QCP with $x = x_c$, which is QCP of FCQPT [7,8,18,20].
For region at sufficiently low temperatures [8,20], that is shown by field, such that at state [8,22,24]. In some cases, for example in HF metal CeRu2Si2, by variation of parameter. The quantum critical line is approaching a quantum critical line (shown by the vertical arrow). The solid line represents the field dependence of the Neél temperature when the AF phase transition is of the first order. The NFL state is characterized by the entropy $S_0$ given by Eq. (5). The horizontal solid arrow represents the direction along which the system transits from the NFL behavior to the LFL one at elevated magnetic field and fixed temperature. The vertical solid arrow represents the direction along which the system transits from the NFL behavior to the LFL one at elevated temperature and fixed magnetic field. The shadowed circle depict the transition temperature $T^*$ from the NFL to LFL behavior.

Schematic phase diagram of the system which is driven to FC by variation of $x$ is reported in Fig. 1. Upon approaching the critical density $x_c$ the system remains in the Landau Fermi liquid (LFL) region at sufficiently low temperatures [8,20], that is shown by the shadow area. At QCP $x_c$ shown by the arrow in Fig. 1, the system demonstrates the NFL behavior down to the lowest temperatures. Beyond the critical point at finite temperatures the behavior is remaining the NFL one and is determined by the temperature-independent entropy $S_0$ [8,27]. In that case at $T \to 0$, the system is approaching a quantum critical line (shown by the vertical arrow and the dashed line in Fig. 1) rather than a quantum critical point. Upon reaching the quantum critical line from the above at $T \to 0$ the system undergoes the first order quantum phase transition, which is FCQPT taking place at $T_{c1} = 0$.

At $T > 0$ the NFL state above the critical line, see Fig. 1, is strongly degenerated, therefore it is captured by the other ones such as superconducting (for example, by the superconducting state in CeCoIn$_5$ [9,24,27]) or by AF state (e.g. AF one in YbRh$_2$Si$_2$ [23]) lifting the degeneracy. The application of magnetic field $B$ $>$ $B_{c0}$ restores the LFL behavior, where $B_{c0}$ is a critical magnetic field, such that at $B$ $>$ $B_{c0}$ the system is driven towards its LFL state [8,22,24]. In some cases, for example in HF metal CeRu$_2$Si$_2, B_{c0} = 0$, see e.g. [31], while in YbRh$_2$Si$_2, B_{c0} \approx 0.06 T$ [32]. In our simple model of homogeneous electron liquid $B_{c0}$ is taken as a parameter.

3. $T$-$B$ phase diagram for YbRh$_2$Si$_2$ versus one for CeCoIn$_5$

In Fig. 2, we present temperature $T/T_N$ versus field $B/B_{c0}$ schematic phase diagram for YbRh$_2$Si$_2$. There $T_N(B)$ is the Néel temperature as a function of the magnetic field $B$. The solid and dash lines indicate boundary of the AF phase at $B/B_{c0} \leq 1$ [32]. For $B/B_{c0} \geq 1$, the dash–dot line marks the upper limit of the observed LFL behavior. This dash–dot line separates the NFL state and the weakly polarized LFL, and is represented by [8]

$$\frac{T^*}{T_N} = a_1 \left( \frac{B}{B_{c0}} \right) - 1, \quad (8)$$

where $a_1$ is a parameter. We note that Eq. (8) is in good agreement with facts [32]. Thus, YbRh$_2$Si$_2$ demonstrates two different LFL states, where the temperature-dependent electrical resistivity $\Delta \rho$ follows the LFL behavior $\Delta \rho \propto T^2$, one being weakly AF ordered ($B \leq B_{c0}$ and $T < T_N(B)$) and the other being weakly polarized ($B > B_{c0}$ and $T < T^*(B)$) [32]. At elevated temperatures and fixed magnetic field the NFL state occurs which is separated from the AF phase by the curve $T_N(B)$ of phase transition. In accordance with experimental facts we assume that at relatively high temperatures $T/T_N(B) < 1$ the AF phase transition is of the second order [1,32]. In that case, the entropy and the other thermodynamic functions are continuous functions at the curve of the phase transitions $T_N(B)$. This means that the entropy of the AF phase $S_{AF}(T)$ coincides with the entropy $S(T)$ of the NFL state

$$S_{AF}(T \to T_N(B)) = S(T \to T_N(B)). \quad (9)$$

Since the AF phase demonstrates the LFL behavior, that is $S_{AF}(T \to 0) \to 0$, Eq. (9) cannot be satisfied at diminishing temperatures $T < T_{c1}$ due to the temperature-independent term $S_0$ given by Eq. (5). Thus, in the NFL region formed by FCQPT the second order AF phase transition inevitably becomes the first order one at the tricritical point with $T = T_{c1}$, as it is shown in Fig. 2. At $T = 0$, the critical field $B_{c0}$ is determined by the condition that the ground state energy of the AF phase coincides with the ground state energy of the weakly polarized LFL and the ground state of YbRh$_2$Si$_2$ becomes degenerated at $B = B_{c0}$. Therefore, the Néel temperature $T_N(B = B_{c0}) \to 0$.

Upon comparing the phase diagram of YbRh$_2$Si$_2$ depicted in Fig. 2 with that of CeCoIn$_5$ shown in Fig. 3, it is possible to conclude that they are similar in many respects. Indeed, the line of the second order superconducting phase transitions changes to the line of the first ones at the tricritical point shown by the square in Fig. 3. This transition takes place under the application of magnetic field $B > B_{c2} \geq B_{c0}$ [9,24], where $B_{c2}$ is the critical field destroying the superconducting state, and $B_{c0}$ is the critical field at which the magnetic field induced QCP takes place [33,34]. We note that the superconducting boundary line $B_{c2}(T)$ at lowering temperatures acquires the tricritical point due to Eq. (9) that cannot be satisfied at diminishing temperatures $T < T_{c1}$, i.e. the corresponding phase transition becomes first order [9,24,33]. This permits us to conclude that at lowering temperatures, in the NFL region formed by FCQPT the curve of any second order phase transition passes into the curve of the first order one at the tricritical point.
4. The tricritical point in the B–T phase diagram of YbRh2Si2

The Landau theory of the second order phase transitions is applicable as the tricritical point is approached, $T \simeq T_{cr}$, since the fluctuation theory can lead only to further logarithmic corrections to the values of the critical indices. Moreover, near the tricritical point, the difference $T_{cr}(B) - T_c$ is a second order small quantity when entering the term defining the divergence of the specific heat [2]. As a result, upon using the Landau theory we obtain that the Sommerfeld coefficient $\gamma_0 = C/T$ varies as $\gamma_0 \propto |t - 1|^{-\alpha}$ where $t = T/T_{cr}(B)$ with the exponent is $\alpha \simeq 0.5$ as the tricritical point is approached at fixed magnetic field [2]. We will see that $\alpha = 0.5$ gives good description of the facts collected in measurements of the specific heat on YbRh2Si2. Taking into account that the specific heat increases in going from the asymmetrical AF phase [2], we obtain

$$\gamma_0(t) = A + \frac{B}{\sqrt{|t - 1|}}. \tag{10}$$

Here, $B = B_{\pm}$ are the proportionality factors which are different for the two sides of the phase transition, the parameters $A = A_\pm$ related to the corresponding specific heat $(C/T)_{\pm}$ are also different for the two sides, and “+” stands for $t > 1$, “−” stands for $t < 1$.

The attempt to fit the available experimental data for $\gamma_0 = C(T)/T$ in YbRh2Si2 at the AF phase transition in zero magnetic fields [1] by the formula (10) is reported in Fig. 4. We show there the normalized Sommerfeld coefficient $\gamma_0/A_\pm$ as a function of the normalized temperature $T/T_{cr}(B = 0)$. It is seen that the normalized Sommerfeld coefficient $\gamma_0/A_\pm$ extracted from $C/T$ measurements on YbRh2Si2 [1] is well described in the entire temperature range around the AF phase transition by the formula (10) with $A_\pm = 1$.

Now transform Eq. (10) to the form

$$\frac{\gamma_0(t) - A}{B} = \frac{1}{\sqrt{|t - 1|}}. \tag{11}$$

It follows from Eq. (11) that the ratios $(\gamma_0 - A)/B$ for $t < 1$ and $t > 1$ versus $|t - 1|$ are to collapse into a single line in logarithmic-logarithmic plot. The extracted from experimental facts [1] ratios are depicted in Fig. 5. Coefficients $A$ and $B$ are taken from the fitting $\gamma_0$ shown in Fig. 4. It is seen from Fig. 5 that the ratios $(\gamma_0 - A)/B$ shown by the upward and downwards triangles for $t < 1$ and $t > 1$ respectively do collapse into the single line shown by the solid straight line.

5. Entropy in YbRh2Si2 at low temperatures

It is instructive to analyze the evolution of magnetic entropy in YbRh2Si2 at low temperatures. We start with considering the derivative of magnetic entropy $dS(B,T)/dB$ as a function of magnetic field $B$ at fixed temperature $T_f$ when the system transits from the NFL behavior to the LFL one as shown by the horizontal

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**Fig. 3.** B–T phase diagram of the CeColn5 heavy fermion metal. The interface between the superconducting and normal phases is shown by the solid and dash lines. At $T < T_{ph}$ the curve of the second order superconducting phase transitions passes into a curve of the first order ones at the tricritical point shown by the square [33]. The interface between the superconducting and normal phases is shown by the dashed line. The solid straight line with the experimental points [34] shown by squares is the interface between the Landau Fermi liquid (LFL) and non-Fermi liquid (NFL) states [9,33,34].

**Fig. 4.** The temperature dependence of the normalized Sommerfeld coefficient $\gamma_0/A_\pm$ as a function of the normalized temperature $t = T/T_{cr}(B = 0)$ given by the formula (10) is shown by the solid line. The normalized Sommerfeld coefficient is extracted from the facts obtained in measurements on YbRh2Si2 at the AF phase transition [1] and shown by the triangles.

**Fig. 5.** The temperature dependence of the ratios $(\gamma_0 - A)/B$ for $t < 1$ and $t > 1$ versus $|t - 1|$ given by the formula (11) is shown by the solid line. The ratios are extracted from the facts obtained in measurements of $\gamma_0$ on YbRh2Si2 at the AF phase transition [1] and depicted by the triangles as shown in the legend.

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A few remarks are in order here. The good fitting shown in Figs. 4 and 5 of the experimental facts by the functions (10) and (11) with the critical exponent $\alpha = 1/2$ allows us to conclude that the specific-heat measurements on YbRh2Si2 [1] are taken near the tricritical point and to predict that the second order AF phase transition in YbRh2Si2 changes to the first order under the application of magnetic field as it is shown by the arrow in Fig. 2. It is seen from Fig. 4 that at $t \simeq 1$ the peak is sharp, while one would expect that anomalies in the specific heat associated with the onset of magnetic order are broad [1,35,36]. Such a behavior presents fingerprints that the phase transition is to be changed to the first order one at the tricritical point, as it is shown in Fig. 2. As seen form Fig. 4, the Sommerfeld coefficient is larger below the phase transition than above it. This fact is in accord with the Landau theory stating that the specific heat is increased when passing from $t > 1$ to $t < 1$ [2].
solid arrow in Fig. 2. Such a behavior is of great importance since exciting experimental facts [37] on measurements of the magnetic entropy in YbRh$_2$Si$_2$ allow us to analyze reliability of the employed theory and to study the scaling behavior of the entropy when the system in its NFL, transition and LFL states.

According to the well-known thermodynamic equality $dM/dT = dS/dB$, and $\Delta M/\Delta T \approx dS/dB$. To carry out a quantitative analysis of the scaling behavior of $dS(B,T)/dB$, we calculate the entropy $S$ as a function of $B$ at fixed temperature $T$ within the model of homogeneous electron liquid taking into account that the electronic system of YbRh$_2$Si$_2$ is located at FCQPT [23]. Fig. 6 reports the normalized $(dS/dB)_N$ as a function of the normalized magnetic field. The normalized function $(dS/dB)_N$ is obtained by normalizing $-dS/dB$ by its maximum taking place at $B_B$, and the field $B$ is scaled by $B_B$. The measurements of $\Delta M/\Delta T$ are normalized in the same way and depicted in Fig. 6 as $(\Delta M/\Delta T)_N$ versus normalized field. It is seen from Fig. 6 that our calculations shown by the solid line are in good agreement with the facts collected on YbRh$_2$Si$_2$ [37]. Our calculation of the normalized derivative $(dS/dB)_N$ versus normalized magnetic field is shown by the solid line.

Now we are in position to evaluate the entropy $S$ at temperatures $T \lesssim T^*$ in YbRh$_2$Si$_2$. At $T < T^*$ the system in its LFL state, the effective mass is independent of $T$, and is a function of magnetic field $B$ [8,32]

\[
M/M_c(B) = \frac{\sqrt{B/B_c} - 1}{a_2},
\]

where $a_2$ is a parameter. In the LFL state at $T < T^*$ when the system moves along the vertical arrow shown in Fig. 2, the entropy is given by the well-known relation, $S = M^* T^* \pi^2/6 = \gamma_0 T$ [17]. Taking into account Eqs. (8) and (12) we obtain that at $T \sim T^*$ the entropy is independent of both magnetic field and temperature, $S(T) \sim \gamma_0 T^* \simeq S_0 \simeq a_1 M^* T^* /a_2 p^2$. Upon using the data [32], we obtain that for fields applied along the hard magnetic direction $S_0(B \parallel c) \sim 0.03 R \ln 2$, and for fields applied along the easy magnetic direction $S_0(B \perp c) \sim 0.005 R \ln 2$. Thus, in accordance with facts collected on YbRh$_2$Si$_2$ [32] we conclude that the entropy contains the temperature-independent part $S_0$ [8,27] which gives rise to the tricritical point.

### 6. Conclusions

We have predicted that the curve of the second order AF phase transitions in YbRh$_2$Si$_2$ passes into the curve of the first order ones at the tricritical point under the application of magnetic field. Moreover, we have shown that in the NFL region formed by FCQPT the curve of any second order phase transition passes into a curve of the first order one at the tricritical point leading to the violation of the critical universality of the fluctuation theory. This change is generated by the temperature-independent entropy $S_0$ formed behind FCQPT. Near the tricritical point the Landau theory of second order phase transitions is applicable and gives the critical index $\alpha = 1/2$. Bearing in mind that a theory is an important input in understanding of what we observe, we demonstrate that this value of $\alpha$ is in good agreement with the specific-heat measurements on YbRh$_2$Si$_2$ [1] and conclude that the critical universality of the fluctuation theory is violated at the AF phase transition [1] since the second order phase transition is about to change to the first order one making $\alpha \rightarrow 1/2$.

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### References