Behavior of second order phase transitions at a quantum critical point

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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 at $T_N = 72$ mK. The corresponding critical exponent $\alpha$ turns out to be $\alpha = 0.38$, which differs significantly from that obtained within the framework of the fluctuation theory of second order phase transitions based on the scale invariance, where $\alpha \simeq 0.1$. We show that under the application of magnetic field the curve of the second order AF phase transitions passes into a curve of the first order ones at the tricritical point leading to a violation of the critical universality of the fluctuation theory. This change of the phase transition is generated by the fermion condensation quantum phase transition. Near the tricritical point the Landau theory of second order phase transitions is applicable and gives $\alpha \simeq 1/2$. We demonstrate that this value of $\alpha$ is in good agreement with the specific-heat measurements.

In this letter, we analyze the specific-heat measurements on YbRh$_2$Si$_2$ in the vicinity of the second order AF phase transition with $T_N = 72$ mK. 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 $\alpha \simeq 0.1$. We show that under the application of magnetic field $B$ the curve $T_N(B)$ 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 $T_{cr} = T_N(B_{cr})$. This change is generated by FCQPT.
Near the tricritical point the Landau theory of second order phase transitions is applicable and gives $\alpha \approx 1/2$\cite{3}. This value of $\alpha$ is in good agreement with the specific-heat measurements. As a result, we conclude that the critical universality of the fluctuation theory is violated at the AF phase transition due to the tricritical point.

We start with visualizing the main properties of FCQPT. To this end, consider the density functional theory for superconductors (SCDFT)\cite{22}. SCDFT states that the thermodynamic potential $\Phi$ is a universal functional of the density $n(r)$ and the anomalous density (or the order parameter) $\kappa(r, r_1)$ and provides a variational principle to determine the densities\cite{22}. 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. In that case, the superconducting state takes place at $T = 0$ while at finite temperatures there is a normal state. This means that in this state the anomalous density is finite while the superconducting gap vanishes. For the sake of simplicity, we consider a homogeneous Fermi (electron) system. Then, the thermodynamic potential reduces to the ground state energy $E$ which turns out to be a functional of the occupation number $n(p)$ since $\kappa = \sqrt{n(1-n)}\, \text{[14, 22, 23, 24]}$. Upon minimizing $E$ with respect to $n(p)$, we obtain

$$\frac{\delta E}{\delta n(p)} = \varepsilon(p) = \mu, \qquad (1)$$

where $\mu$ is the chemical potential. It is seen from Eq. (1) that instead of the Fermi step, we have $0 \leq n(p) \leq 1$ in certain range of momenta $p_s \leq p \leq p_F$ with $\kappa$ is finite in this range. Thus, the step-like Fermi filling inevitably undergoes restructuring and forms the fermion condensate (FC) as soon as Eq. (1) possesses non-trivial solutions at some point $x = x_c$ when $p_1 = p_F$\cite{14, 16}. Here $p_F$ is the Fermi momentum and $x = p_F/3\pi^2$.

At any small but finite temperature the anomalous density $\kappa$ (or the order parameter) decays and this state undergoes the first order phase transition and converts into a normal state characterized by the thermodynamic potential $\Phi_0$. At $T \to 0$, the entropy $S = -\partial \Phi_0/\partial T$ of the normal state is given by the well-known relation\cite{13}

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

which follows from combinatorial reasoning. Since the entropy of the superconducting ground state is zero, it follows from Eq. (2) that the entropy is discontinuous at the phase transition point, with its discontinuity $\Delta S = S_0$. The heat $q$ of transition from the asymmetrical to the symmetrical phase is $q = T_c$ $S_0 = 0$ since $T_c = 0$. 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\cite{13}

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

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. (3) reads\cite{25, 26}

$$\frac{M^*}{M} = \frac{1}{1 - N_0 F^3(x)/3}. \qquad (4)$$

Here $N_0$ is the density of states of a free electron gas and $F^3(x)$ is the $p$-wave component of Landau interaction amplitude $F$. When at some critical point $x = x_c$, $F^3(x)$ achieves certain threshold value, the denominator in Eq. (4) tends to zero so that the effective mass diverges at $T = 0$\cite{25, 26}. It follows from Eq. (4) 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, the system must undergo a quantum phase transition at the quantum critical point $x = x_c$, which is FCQPT\cite{2, 4, 14, 16}.

![FIG. 1: Schematic phase diagram of the system driven to the FC state. The number density $x$ is taken as the control parameter and depicted as $x/x_c$. The quantum critical point, $x/x_c = 1$, of FCQPT is shown by the arrow. At $x/x_c < 1$ and sufficiently low temperatures, the system in the Landau Fermi liquid (LFL) state as shown by the shadow area. At $T = 0$ and beyond the critical point, $x/x_c > 1$, the system is at the quantum critical line depicted by the dash line and shown by the vertical arrow. The critical line is characterized by the FC state with finite superconducting order parameter $\kappa$. At $T_c = 0$, $\kappa$ is destroyed, the system undergoes the first order phase transition and exhibits the NFL behavior at $T > 0$.](image-url)
LFL region at sufficiently low temperatures \[4, 16\], that is shown by the shadow area. At the quantum critical point \(x_c\) 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 \(S_0\) \[23\]. 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 \(T_c = 0\).

At \(T > 0\) the NFL state above the critical line, see Fig. 1 is strongly degenerated, therefore it is captured by the other states such as superconducting (for example, by the superconducting state in CeCoIn\(_5\) \[5, 20, 23\]) or by AF state (e.g. AF one in YbRh\(_2\)Si\(_2\) \[19\]) 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 Landau Fermi liquid (NFL) regime \[20\]. In some cases, for example in HF metal CeRu\(_2\)Si\(_2\), \(B_{c0} = 0\), see e.g. \[27\], while in YbRh\(_2\)Si\(_2\), \(B_{c0} \approx 0.06\ T\) \[28\]. In our simple model \(B_{c0}\) is taken as a parameter.

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 dash and solid lines indicate boundary of the AF phase at \(B/B_{c0} \leq 1\) \[28\]. For \(B/B_{c0} \geq 1\), the dash-dot line marks the upper limit of the observed LFL behavior. 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 \((B \leq B_{c0} \text{ and } T < T_N(B))\) and the other being weakly polarized \((B \geq B_{c0} \text{ and } T < T^*(B))\) \[28\]. At elevated temperatures and fixed magnetic field the NFL regime 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 \(T/T_N(B) \approx 1\) the AF phase transition is of the second order \[1, 28\]. 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

\[
S_{AF}(T \to T_N(B)) = S(T \to T_N(B)).
\]  

Since the AF phase demonstrates the LFL behavior, that is \(S_{AF}(T \to 0) \to 0\), Eq. 5 cannot be satisfied at diminishing temperatures \(T \leq T_{cr}\) due to the temperature-independent term \(S_0\) given by Eq. 2. Thus, the second order AF phase transition becomes the first order one at \(T = T_{cr}\) 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 \(T_N(B \to B_{c0}) \to 0\).
ond order phase transitions is applicable at the tricritical point \( T \approx T_{cr} \) since the fluctuation theory can lead only to further logarithmic corrections to the values of the critical indices \( ^2 \). As a result, upon using the Landau theory we obtain that the Sommerfeld coefficient \( \gamma_0 = C/T \) varies as \( \gamma_0 \propto 1/\sqrt{|t-1|} \) as the tricritical point is approached at fixed magnetic field \( ^2 \), where \( t = T/T_N(B) \).

Taking into account that the specific heat increases in going from the symmetrical to the asymmetrical AF phase \( ^2 \), we obtain

\[
\gamma_0(t) = A_0 + \frac{B_0}{\sqrt{|t-1|}}
\]  

(6)

Here, \( B_0 \) are the proportionality factors which are different for the two sides of the phase transition, the parameters \( A_0 \) related to the corresponding specific heat \( (C/T)_0 \) are also different for the two sides, and \( \pm \) stands for \( t > 1 \), \( - \) stands for \( t < 1 \).

The attempt to fit the available experimental data for \( \gamma_0 = C(T)/T \) in YbRh\(_2\)Si\(_2\) at the AF phase transition in zero magnetic fields \( ^1 \) by the formula \( ^6 \) is reported in Fig. 3. We show there the normalized Sommerfeld coefficient \( \gamma_0/A_0 \) as a function of the normalized temperature \( T/T_N(B=0) \). It is seen that the normalized Sommerfeld coefficient \( \gamma_0/A_0 \) extracted from \( C/T \) measurements on YbRh\(_2\)Si\(_2\) \( ^1 \) can be well described by the formula \( ^6 \) with \( A_0 = 1 \).

A few remarks are in order here. The good fitting of the experimental facts by the function \( ^6 \) with the critical exponent \( \alpha = 1/2 \) allows us to predict that the second order AF phase transition in YbRh\(_2\)Si\(_2\) changes to the first order under the application of magnetic field as it is shown by the arrow in Fig. 2.