YbRh$_2$Si$_2$: Quantum tricritical behavior in itinerant electron systems

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We propose that proximity of the first-order transition manifested by the quantum tricritical point (QTCP) explains non-Fermi-liquid properties of YbRh$_2$Si$_2$. Here, at the QTCP, a continuous phase transition changes into first order at zero temperature. The non-Fermi-liquid behaviors of YbRh$_2$Si$_2$ are puzzling in two aspects; diverging ferromagnetic susceptibility at the antiferromagnetic transition and unconventional power-law dependence in thermodynamic quantities. These puzzles are solved by an unconventional criticality derived from our spin fluctuation theory for the QTCP.

KEYWORDS: quantum critical phenomena, quantum tricritical point, YbRh$_2$Si$_2$, non-Fermi-liquid behavior, self-consistent renormalization theory

Critical temperatures of the symmetry-breaking phase transitions can be lowered to zero at the quantum critical point (QCP) by tuning quantum fluctuations such as by magnetic fields as shown in Fig. 1(a). Quantum critical phenomena in metals have attracted much interest from both theoretical and experimental points of view, because of not only its own right but also unconventional superconductivity as well as non-Fermi-liquid behavior observed near the QCP.\textsuperscript{1,2}

The conventional spin fluctuation theory of the QCP by Moriya, Hertz and Millis\textsuperscript{2–5} has succeeded in explaining a number of non-Fermi-liquid properties. However, this picture has been challenged by many recent experiments,\textsuperscript{1,2,6} where criticalities of thermodynamic and transport properties do not follow it.

A typical heavy-fermion compound YbRh$_2$Si$_2$\textsuperscript{1} belongs to such an unconventional category. At the magnetic field $H = 0$, it exhibits an antiferromagnetic (AF) transition at the Néel temperature $T_N = 0.07$K. An AF QCP emerges at the critical magnetic field $H_c \sim 0.06$T along the $c$ axis.\textsuperscript{7,8} Near $H_c$, Sommerfeld coefficient of specific heat $\gamma$ is logarithmically increased with lowering temperature $T$ above 0.3K and even faster below it\textsuperscript{9} in contrast to the conventional theory predicting convergence to a constant. Transport and optical data roughly show the resistivity linearly scaled with $T$ and frequency.\textsuperscript{7} Among all, a key aspect is an unusually enhanced ferromagnetic susceptibility $\chi_0$ roughly scaled by $\chi_0 \propto T^{-\zeta}$ and $\chi_0 \propto |H - H_c|^{-\zeta'}$ with $\zeta \sim \zeta' \sim 0.6^8$ contradicting the standard expectation of saturation to a constant. In accordance, the magnetization shows convex dependence on $H$.\textsuperscript{8} NMR\textsuperscript{10} and ESR\textsuperscript{11} signals are also consistent. These non-Fermi-liquid properties are all contradicting the standard theory\textsuperscript{2–5} for the AF QCP and are under extensive debates.\textsuperscript{5}

A hint comes from the fact that the first-order transition is observed for YbRh$_2$Si$_2$ under pressure.\textsuperscript{12} Actually, the proximity of the first-order transition is common in many compounds with unconventional non-Fermi-liquid properties. Our idea is that the proximity of the first-order transition, namely, tricriticality solves the puzzle because the tricriticality necessarily induces ferromagnetic tendency even at a clear AF transition.

At $T \neq 0$, the tricritical point (TCP) where phase transitions change from continuous to first order as in Fig. 1 (b) has been studied in detail.\textsuperscript{13} A characteristic feature of TCP is the diverging susceptibility not only at the ordering wavenumber $Q$ but also at zero ($\chi_0$).\textsuperscript{14}

If quantum fluctuations suppress the temperature of TCP to zero, quantum tricritical point (QTCP) appears [see Fig. 1(c)]. Then QTCP may alter the criticality of QCP as a proximity of the first-order transition.

Recently TCP has been studied for the itinerant ferromagnet to understand the nature of the global phase

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diagram of weak itinerant ferromagnets ZrZn$_2$ and UGe$_2$. Furthermore, ferromagnetic QTCP has been studied for itinerant helical ferromagnet MnSi$^{16}$ and nearly ferromagnetic metal Sr$_3$Ru$_2$O$_7$. However, these previous studies on the ferromagnetic QTCP do not explain the unconventional coexistence of the ferromagnetic and AF fluctuations observed near the AF QCP in YbRh$_2$Si$_2$.

In this letter, we propose that the proximity of the first-order transition opens a way to solve the puzzles in the AF quantum critical phenomena. The proximity of the first-order transition inherently generates diverging ferromagnetic fluctuations concomitantly with the order-parameter (AF) fluctuations. The emergence of the concomitance is manifested by the quantum tricriticality, which generates an unexplored non-Fermi liquid. An unconventional scaling is derived by extending the self-consistent renormalization (SCR) theory$^3$ for spin fluctuations. Our result accounts for the otherwise puzzling properties of YbRh$_2$Si$_2$, even when we do not consider the possible valence transitions$^{18}$ or collapse of $f$-electron itinerancy as in the picture of the local quantum criticality.$^{19}$

To understand the QTCP, we start from a standard Ginzburg-Landau-Wilson (GLW) expansion effective action for bozonic spin fields $\varphi_i$ at the wave number $q$,$^{3-5}$

$$S[\varphi_i] = \frac{1}{2} \sum_{q} r_q |\varphi_i|^2 + \sum_{q, q', q''} u(q, q', q'') (\varphi_{i} \cdot \varphi_{i-q'})$$

$$\times (\varphi_{i-q'} \cdot \varphi_{i-q-q''}) + v \sum_{q \approx q_0} (\varphi_{q_1} \cdot \varphi_{q_2}) (\varphi_{q_3} \cdot \varphi_{q_4})$$

$$\times (\varphi_{q_1} \cdot \varphi_{q_2} + \varphi_{q_3} - \varphi_{q_4}) - H \varphi_i,$$  

(1)

where $H$ is external magnetic field; $u(q, q', q'')$ and $v$ are constants, while $r_q$ depends on the magnetic field $H$. From eq. (1), the free energy $F$ is obtained from

$$\exp(-F/T) = \prod_q D\varphi_i \exp(-S[\varphi_i]/T).$$  

(2)

Since the QTCP is expressed by fluctuations at both the order parameter $M_1 = \langle \varphi_i \rangle$ and the uniform magnetization $M = \langle \varphi_i \rangle$:

$$F_0 = \frac{1}{2} r_i M_1^2 + \tilde{u}_i M_1^4 + v M_1^6$$

$$+ \frac{1}{2} r_0 M_2^2 + \tilde{u}_0 M_4^4 + v M_6^6 - H M,$$  

(3)

where $\tilde{r}_i$, $\tilde{u}_i$, $\tilde{u}_0$, and $\tilde{K}$ are defined as

$$\tilde{r}_i(T, H) = r_i (H) + 12 u_i(K + M^2) + 90 v(K + M^2)^2, \tilde{u}_i(T, H) = u_i + 15 v(K + M^2), \tilde{u}_0(T, H) = u_0 + 15 v K,$$

$$\tilde{K} = \sum_{q \neq 0} \langle |\varphi_i|^2 \rangle.$$  

(4)

Effects of spin fluctuations are included in $\tilde{K}$ following the SCR theory. We approximate $u(q, q, Q)$ $[u(q, q, 0)]$ and the equivalent coefficients as $q$-independent values; $u(q, q, Q) \approx u_0 [u(q, q, 0) \approx u_0]$ for all $q$ [for $q \neq Q$].

We eliminate $M$ in eq. (3) by using the saddle point condition for $M$, $\partial F_0/\partial M = 0$ leading to the relation between $M$ and $M_1$ as

$$M = a_0 + a_1 M_1^2 + a_2 M_1^4 + \cdots,$$  

(5)

where the expansion coefficients $a_0 \sim a_2$ are determined by substituting eq. (5) into the saddle point condition:

$$\tilde{r}_i(T, H) a_0 + 4 \tilde{u}_i(T, H) a_0^3 + 6 v a_0^5 - H = 0,$$  

(6)

$$12 a_0 \tilde{u}_0(T, H) + a_1 R(T, H) = 0,$$  

(7)

where $R(T, H) = \tilde{r}_i(T, H) + 12 \tilde{u}_i(T, H) a_0^2 + 30 v a_0^4$. By using eq. (5), we obtain the free energy as

$$F_0 = \frac{1}{2} r_i Q(T) M_1^2 + \tilde{u}_i Q(T, H) M_1^4 + O(M_6^6),$$  

(8)

where $\tilde{u}_i Q(T, H) = \tilde{u}_i Q(T, H) (1 + 6 a_0 a_1)$. In eq. (8), continuous phase transitions occur at $\tilde{r}_i = 0$ when $\tilde{u}_i Q(T, H) > 0$, while the first-order phase transitions occur when $\tilde{u}_i Q(T, H) < 0$. Therefore, the QTCP appears when the conditions $\tilde{r}_0 (H_1) = 0$ and $\tilde{u}_0 (H_1) = 0$ are both satisfied,$^{20}$ where $H_1$ is the critical field at the QTCP.

We now discuss the susceptibilities $\chi_i$ at the AF vector $Q$ and $\chi_0$ at $q = 0$ in the disordered phase ($M = a_0$) by using eq. (6) and the free energy (8). From eq. (8), $\chi_i^{-1}$ is given as

$$\chi_i^{-1} = \frac{\partial^2 F_0}{\partial M_1^2} \bigg|_{M = 0} = \tilde{r}_i Q(T, H).$$  

(9)

By differentiating eq. (6) with respect to the magnetic field $H$, we obtain $\chi_0^{-1}$ as

$$\chi_0^{-1} = (\frac{\partial a_0}{\partial H})^{-1} = \frac{R(T, H)}{1 - a_0 \partial r_0 / \partial H - 4 a_0^2 \partial \tilde{u}_0 / \partial H} \in \tilde{u}_0 Q(T, H).$$  

(10)

Here, we used eq. (7), which gives $R(T, H) \propto \tilde{u}_0 Q(T, H)$. Now, the fluctuation-dissipation (FD) theorem$^{21}$

$$\sum_{q \neq 0} \langle |\varphi_i|^2 \rangle = \frac{2}{\pi} \int_0^\infty d\omega \left[ \phi^2 + n(\omega) \right] \sum_{q \neq 0} \text{Im} \chi(q, \omega),$$  

(11)

and $n(\omega) \equiv 1/(e^{\omega/T} - 1)$, combined with eqs. (4), (6), (9), and (10) constitute the self-consistent equations to determine $K$ and $\chi$ in the scheme of our extended SCR theory. Using this SCR theory, we now clarify how the susceptibilities and the magnetization measured from the QTCP ($\chi_0^{-1}$, $\chi_i^{-1}$, $\delta a_0 \equiv a_0 - a_0$ with $a_0$ being the value at the QTCP) are scaled with $\delta H = H - H_1$ and $T$ near the QTCP. The results will be shown in eqs. (15)-(17).

In the SCR theory, non-trivial temperature dependence of physical properties comes from the spin fluctuation term $K$. Therefore, we first clarify the scaling of $K$ by using the FD theorem combined with expansions of $\chi_{0+q}(\omega)$ and $\chi_{Q+q}(\omega)$ in terms of the wavevector $q$ and the frequency $\omega$ near the QTCP. The ordering susceptibility $\chi_{Q+q}(\omega)$ is assumed to follow the conventional Ornstein-Zernike form $\chi_{Q+q}(\omega) \sim \chi_0^{1} + A q^2 - i C Q \omega$ as in the SCR formalism, while the uniform form $\chi_{0+q}(\omega)$ turns out to not follow. This is because the scaling relation $\chi_0^{-1} \sim \chi_0^{1/2}$ holds near TCP within the GLW theory.$^{13}$ As we will see, the self-consistency among eqs. (4), (6), (9), (10), and (11) requires that this relation still holds for $q \neq 0$. Therefore,
we obtain the relation as \( \chi_{0+}(0)^{-1} \propto (\chi_{0+}^{-1} + Aq_0 q^2)^{1/2} \propto (\chi_{0+}^{-1} + Aq_0 q^2)^{1/2} \). From the conservation law, \( \omega \) dependence of \( \chi_{0+}(0)^{-1} \) should be given as \( \chi_{0+}(\omega)^{-1} \approx \chi_{0+}(0)^{-1} - i \delta \omega / q \). Finally, we obtain \( \omega \) and \( q \) expansions of \( \chi_{0+}(\omega)^{-1} \) as 
\[
(\chi_{0+}^{-1} + Aq_0 q^2)^{1/2} \propto -i \delta \omega / q.
\]

By substituting the above forms for \( \chi_{0+}(\omega)^{-1} \) into the FD theorem (11), the contributions from the spin fluctuations near zero (ordering) wavenumber is given as
\[
\sum_{q \to 0} (\xi_q^2)^2 \approx K_{00} - K_{01} \chi_{01}^{-1} + K_{0T} T^2 - K_{QT} T^3/2,
\]
\[
\sum_{q \to 0} (\xi_q^2)^2 \approx K_0 - K_{Q1} \chi_{Q1}^{-1} + K_{QT} T^3/2\text{ where } K_0, K_{Q1}, K_{QT}, K_{Q1}, \text{ and } K_{QT} \text{ are constants. From these relations, in three dimensions, we obtain the scaling of } \delta K \text{ measured from the QTCP as}
\]
\[
\delta K \approx -K_{01} \chi_{01}^{-1} - K_{Q1} \chi_{Q1}^{-1} + K_{QT} T^2 + K_{QT} T^3/2.
\]

The singularity of magnetization \( a_0 \) is given as solving eq. (6). Near the QTCP, eq. (6) can be approximated as
\[
A \delta a_0^2 + 2B \delta a_0 + C = 0,
\]
with \( A = 12a_0 (\beta_a a_0 + \tilde{w}_0), B = \delta t + 12a_0 \delta \tilde{w}_0, \) and \( C = a_0 \delta \tilde{t} + 4a_0^2 \delta^2 - \delta H, \) where \( \delta \tilde{t} = \tilde{t}(0, H), \) and \( \delta \tilde{w}_0 = \tilde{w}_0(T, H) - \tilde{w}_0(0, H). \) Since both \( B \) and \( C \) vanish at the QTCP, we obtain the asymptotic behavior of \( \delta a_0 \) as
\[
\delta a_0 \approx (\alpha_0 \delta H + \alpha_1 \delta K)^{1/2},
\]
where \( \alpha_0, \alpha_1 \) are constants.

By defining \( \delta Q = r_{Q}(T, H) - \tilde{r}_{Q}(0, H), \) we get
\[
\chi_Q^{-1} = \delta r_{Q}(T, H) \approx r_{Q}(H) + 90v(\delta H + \delta a_0)^2,
\]
while both \( r_{Q}(0, H) \) and \( \tilde{a}_0(0, H) \) are zero at the QTCP and terms linear in \( \delta K \) and \( \delta a_0 \) vanish. Here \( \delta r_Q \) and \( \delta a_0 \) are defined as \( \delta Q = r_{Q}(H) - r_{Q}(H) \approx r_{Q}(H) \delta H, \) \( \delta a_0 = a_0^0 - a_0, \) where \( a_0 \) is determined from the condition \( r_{Q}(0, H) = 0, \) and \( a_0 \) is fixed, the other parameters \( (r_{Q}, r_{Q}, a_0) \) are determined from the conditions \( r_{Q}(0, H) = 0, \) and \( a_0 = 0, \) and eqs. (6), (7). In this letter, to calculate physical properties, we employ a reasonable set of parameters given in ref. 23 as follows: We estimate \( H_t \) and \( a_0 \) directly from experiments and also choose conventional SCR parameters \( (T_0, T_00, T_{Q1}, T_{Q2}) \) within the order of 10-100K. This range of SCR parameters is typical in heavy fermion compounds. In contrast to these, for the other non-principal parameters \( (r_{Q}, r_{Q}, \text{ and } v) \), we do not find any constraint from physical requirement. Therefore, we have freely tuned these parameters to reproduce the experimental results quantitatively. However, the critical exponents do not change even if we have chosen these parameters arbitrarily. Microscopic derivation of these phenomenological parameters is left for future studies.

In Fig. 3 (a), the numerical result of the temperature dependence of \( \chi_0^{-1} \) just on the QTCP is compared with the experimental \( \chi_0^{-1} \) reported in ref. 8. Although we obtain the critical exponent \( \zeta = 0.75 \) (\( \chi_0^{-1} \propto T^{\delta} \)) for \( T \to 0 \), the numerical result shows that \( \chi_0^{-1} \) is roughly scaled by \( T^{0.6} \) at higher temperatures \( (T > 1.0K) \). We emphasize that the puzzling convex behavior of \( \chi_0^{-1} \) for YbRhSi_2 near the QCP can not be accounted for by the conventional quantum criticality, because the critical exponent \( \zeta \) is always larger than one for the conventional quantum critical point. The nonzero offset of experimental \( \chi_0^{-1} \) at \( T = 0 \) indicates that the QCP in YbRhSi_2 (Si_0.95 Ge_0.05) exists slightly away from the QCP. It is an intriguing experimental challenge to determine the precise location of the QTCP by tuning the pressure and the magnetic field.

In Fig. 3 (b), the numerical result of magnetization curve at \( T = 0 \) is compared with the experimental result reported in ref. 8. By using the same parameters, it is noteworthy that not only the uniform susceptibility but also the magnetization is consistent with the experimental result quantitatively in the relevant parameter region. Because the experimentally observed QCP is
In summary, a non-Fermi liquid different from that obtained from the conventional QCP is shown to emerge when the proximity of the first-order transition is involved through the QTCP. The unconventional criticality thus obtained by the extension of the SCR theory solves the puzzles in the experimental results of YbRh$_2$Si$_2$. It is intriguing to examine whether this proximity also plays roles in other unconventional non-Fermi liquids.

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