Magnetically robust non-fermi liquid behavior due to the competition between crystalline-electric field singlet and Kondo-Yosida singlet in f²-based heavy fermion systems

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Abstract. In f²-based heavy fermion systems with a tetragonal symmetry, we investigate the magnetic field dependence of a non-fermi liquid (NFL) which arises related to the quantum critical point (QCP) due to the competition between the crystalline-electric field (CEF) singlet and the Kondo-Yosida singlet states. On the basis of the Wilson numerical renormalization group method, we find that the magnetic field less than a characteristic magnetic field \( H_z \) does not affect the characteristic temperature \( T_F \) at which the specific heat takes a maximum value. Since such \( H_z \) increases as the deviation from the QCP increases, slightly off the QCP, there are parameter regions where NFL behaviors are robust at an observable temperature range \( T > T_F \) against a magnetic field of up to \( H_z \) which is far larger than \( T_F \). Our result suggests that such robust NFL behaviors can arise also in systems with other CEF symmetries; e.g., magnetically robust NFL behaviors observed in UBe₁₃ may be understood on this basis.

1. Introduction
The competition between the crystalline-electric field (CEF) singlet and the Kondo-Yosida (KY) singlet states in f²-based heavy fermion systems has attracted attention. The former one is caused by a localized character of the f-electron, while the latter one is caused by the itinerant character of the f-electron due to the hybridization between the f-electron and conduction electrons. Because of these conflicting characters of the f-electron, the competition of these singlet states causes the quantum critical point (QCP) where the system exhibits non-Fermi liquid (NFL) behaviors similar to the two-channel Kondo model (TCKM) [1]. It is known that properties of Th₁₋ₓUₓRu₂Si₂ [2], and some Pr-based filled skutterudite compounds can be explained on the basis of this NFL [3, 4]. However, the magnetic field effect on this NFL has not been fully studied so far.

In this paper, we investigate the magnetic field dependence of this NFL in a tetragonal symmetry on the basis of the Wilson numerical renormalization group method (NRG) [5, 6, 7]. As in [2], its competition suppresses the characteristic temperature \( T_F \) where the specific heat takes a maximum value compared to the energy scale of each singlet state, \( T_{K2} \) (the lower Kondo temperature) and \( \Delta \) (the CEF splitting for first excited state). In this case, NFL behaviors appear at \( T_F < T < \min(T_{K2}, \Delta) \) as in the case of the TCKM. We demonstrate that \( T_F \) is not affected by the magnetic field less than the characteristic magnetic field \( H^*_z \) which depends on the distance from the QCP. In such a case, there is little change in NFL behaviors under...
and ∆ is related to coupling constants in the Hamiltonian (1) as $J_\perp = K$ and $J_z = 2\Delta - K$, respectively.

Figure 2. $\Delta$ dependence of $T_F^a$ for various magnetic fields, $H_z$. The dashed line represents the critical point where two ground states exchange.

2. Numerical Results and Discussion

We use the two-orbital impurity Anderson model as an appropriate one for treating the present problem. It has already been known that the $f^2$-CEF level scheme in the tetragonal symmetry can be reproduced by introducing an anisotropic “antiferromagnetic Hund’s-rule coupling” [2]. Then, the Hamiltonian is given as follows:

$$
H = \sum_{m\alpha} \varepsilon_{km} c_{km\sigma}^\dagger c_{km\sigma} + \sum_{m\alpha} E_{fkm} f_{m\alpha}^\dagger f_{m\alpha} + \sum_{m} U_m f_{m1}^\dagger f_{m1}^\dagger f_{m1} f_{m1} + \sum_{m\kappa\sigma} \left[ V_{m\kappa} f_{m\sigma}^\dagger c_{m\kappa\sigma} + \text{h.c.} \right] + \frac{J_\perp}{2} \left[ S_1^+ S_2^- + S_1^- S_2^+ \right] + J_z S_1^z S_2^z,
$$

where $f_{m\sigma}^\dagger$ is a creation operator of the f-electron on the orbital $m (= 1, 2)$ with the energy $E_{fkm}$, and its pseudospin operator is $\vec{S}_m$; $c_{m\kappa\sigma}^\dagger$ is a creation operator of the conduction electron with the wave vector $\vec{k}$ hybridizing with the f-electron of the orbital $m$ with the strength $V_{m\kappa}$. We explicitly consider the on-site intra-orbital Coulomb repulsion $U_m$, while other Coulomb repulsion terms are implicitly included in the “antiferromagnetic Hund’s-rule coupling” of which coupling constants are related to $f^2$-CEF level splittings as shown in Fig.1. The hybridizations are set to be isotropic in the momentum space (i.e., $V_{m\kappa} \equiv V_m$), and the conduction bands to be symmetric in the energy space (with an extent from $-D$ to $D$) about a Fermi level. We perform NRG calculations by taking the discretization parameter as $\Lambda = 3.0$, and keeping states up to 1500 states in each iteration step.

The system described by the Hamiltonian (1) shows the competition between the K-Y singlet and the $f^2$-CEF singlet states. There exists two stable fixed points corresponding to these singlet states, and an unstable fixed point between those around where NFL behaviors appear. In the present paper, we take the parameter set in the Hamiltonian (1) as $E_{f1} = E_{f2} = -0.4$, $U_1 = U_2 = 1.0$, $V_1 = 0.45$, $V_2 = 0.3$, $K = 0.16$ measured in unit of $D$, and change the CEF

![Figure 1. $f^2$-CEF level scheme. $K$ and $\Delta$ is related to coupling constants in the Hamiltonian (1) as $J_\perp = K$ and $J_z = 2\Delta - K$, respectively.](image1)

![Figure 2. $\Delta$ dependence of $T_F^a$ for various magnetic fields, $H_z$. The dashed line represents the critical point where two ground states exchange.](image2)
splitting $\Delta$. The energy scale of the K-Y singlet state is given by the lower Kondo temperature $T_{K2} = 6.01 \times 10^{-3}$ which is obtained by a Wilson’s definition, $4T_{K2}(T = 0) = 0.413$. In the case of $K = \Delta = 0$, although, precisely speaking, the actual lower Kondo temperature is different from $T_{K2}$ due to the CEF effect. On the other hand, the energy scale of the $f^2$-CEF singlet state is given by $\min(K, \Delta)$. The competition between the K-Y singlet and the CEF singlet states arises around the point where these two characteristic energies are about the same.

First, we focus on the magnetic field dependence of the characteristic temperature $T_F^*$ at which the specific heat of $f$-electrons, $C_{imp} = \partial S_{imp}(T) / \partial (\log T)$, takes a maximum value just before the entropy, $S_{imp}(T)$, approaching 0 as $T \to 0$. Here, the effect of the magnetic field is taken into account through the Zeeman term, $H_z = -g\mu_B H z_j z$ for $f^1$ states with $j = 5/2$ and $g = 6/7$. That on $f^2$ states also arises by Zeeman term for each $f^1$ orbitals composing $f^2$-states, and the off-diagonal matrix element between $\Gamma_3$ and $\Gamma_4$ singlet states. Fig.2 shows the $\Delta$ dependence of $T_F^*$ under various magnetic fields, $H_z$. For $H_z = 0$, at a critical point $\Delta \equiv \Delta^* \approx 0.112$, one can see that $T_F^*$ is sharply suppressed. This is because $T_F^*$ is given by the energy splitting between two singlet states which are nearly degenerated, not by the characteristic energies of each singlet state, $T_{K2}$ and $\Delta$, near $\Delta \sim \Delta^*$. As the distance from $\Delta^*$ increases, $T_F^*$ asymptotically approaches those of each singlet state: i.e., $T_F^* \approx T_{K2}$ for $\Delta \ll \Delta^*$, and $T_F^* \approx K$ for $\Delta \gg \Delta^*$. On the other hand, the magnetic field dependence of $T_F^*(H_z)$ is hard to see from Fig.2.

Second, in order to see this point, we show the magnetic field dependence of $T_F^*$ near the critical point for $\Delta < \Delta^*$ (the K-Y singlet ground state region) in Fig.3. It is noted that we only show results for $\Delta < \Delta^*$ in this paper, although similar behaviors are observed for $\Delta > \Delta^*$ i.e., in the CEF singlet ground state region. As one can see, $T_F^*(H_z)$ remains constant for $H_z$ less than the characteristic magnetic field $H_z^*$ (as shown by arrows in Fig.3) which is defined approximately as that where $T_F^*$ starts to increase as $H_z$ increases. As the distance from the critical point increases, $H_z^*$ increases. Therefore, $H_z^*$ is considered to be determined by two effects which break the criticality of the TCKM-type NFL fixed point. One is the distance of $\Delta$ from $\Delta^*$, and the other is the magnetic field which breaks the degeneracy of the two singlet

**Figure 3.** Magnetic field dependence of $T_F^*$ around the critical point in the case of the K-Y singlet ground state. Arrows indicate the characteristic magnetic field $H_z^*$.

**Figure 4.** Sommerfeld coefficient $C_{imp}/T$ vs $T$ under various magnetic fields, for (a)$\Delta = 0.112$ and (b)0.106.
states which gives rise to the residual entropy \( S_{\text{imp}}(T = 0) = 0.5 \log 2 \) as in the case of the NFL state in TCKM. In other words, \( H^*_z \) corresponds to the energy scale characterizing a crossover from the TCKM-type NFL fixed point to the polarized local Fermi liquid fixed point.

It is remarked that the magnetic field affects two singlet states. However, since \( H_z(< H^*_z) \) is much smaller than \( T_{K2} \) and \( \Delta \), the magnetic field is essentially considered not to break each singlet state. This means that \( H^*_z \) is not determined by the magnetic field dependence of two singlet states in this case.

Finally, in Fig.4, we show the temperature dependence of the Sommerfeld coefficient \( \gamma_{\text{imp}}(T) \equiv C_{\text{imp}}/T \) for (a)\( \Delta = 0.112 \approx \Delta^* \) and (b)\( \Delta = 0.106 \) under various magnetic fields. In the case of (a), extremely close to the critical point, \( \gamma_{\text{imp}}(T) \) increases as \( H_z \) increases. This is attributed to the drastic increase of \( T_{\text{F}z}(H_z) \), especially in the 10\(^{-4}\) to 10\(^{-3}\) range of the magnetic field. As a result, \( \gamma_{\text{imp}}(T) \) logarithmically increases as \( T \) decreases down to 10\(^{-5}\). On the other hand, in the case of (b), slightly off the critical point, the logarithmic divergence of \( \gamma_{\text{imp}}(T) \) is robust against a magnetic field of up to \( H_z \sim 1.0 \times 10^{-3} \) for \( T > 3 \times 10^{-5} \). However, that is suppressed for \( H_z = 2.0 \times 10^{-3} \). As shown in Fig.3, \( T_{\text{F}z} \) remains constant of up to \( H_z = H^*_z \sim 2 \times 10^{-4} \), and increases rather moderately as \( H_z \) increases below \( H_z \sim 10^{-3} \). This is why the temperature dependence of \( \gamma_{\text{imp}}(T) \) remains the same as that at \( H_z = 0 \) for \( T > 3 \times 10^{-5} \) up to \( H_z \sim 10^{-3} \).

3. Conclusion and Discussion

In conclusion, we have investigated the effect of the magnetic field effect on NFL behaviors due to the competition between the K-Y singlet and the CEF singlet states in \( f^2 \)-based heavy fermion systems with the tetragonal symmetry. Near the critical point, \( T_{\text{F}z} \) has been shown not to be affected by the magnetic field less than the characteristic magnetic field \( H^*_z \). We demonstrated that, in the vicinity of the QCP, there are parameter regions where the NFL behavior of the Sommerfeld coefficient is robust against the magnetic field of up to \( H_z \sim H^*_z \). This is because such \( H^*_z \) increases as the system deviating from the QCP.

We expect that such an effect of the competition also causes the NFL behavior similar to the present one in systems with other CEF symmetries. UBe\(_{13}\), a cubic heavy fermion system, is considered to be one of its candidates because of the experimental result indicating the competition between the K-Y singlet and the CEF singlets \[9\]. A detailed report will be published elsewhere. Although all the results in this paper are for the \( f^2 \)-impurity problem, the effect of the competition can play an important role also in lattice systems to exhibit such a NFL robust against the magnetic field because the contribution to the Sommerfeld coefficient from the competition is known to be large \[2, 4\].

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