Grüneisen ratio at the Kondo breakdown quantum critical point

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We show that the scenario of multi-scale Kondo breakdown quantum critical point (QCP) gives rise to a divergent Grüneisen ratio with an anomalous exponent 0.7. In particular, we fit the experimental data of $YbRh_2(Si_{0.95}Gd_{0.05})_2$ for specific heat, thermal expansion, and Grüneisen ratio based on our simple analytic expressions. A reasonable agreement between the experiment and theory is found for the temperature range between 0.4 K and 10 K. We discuss how the Grüneisen ratio is a key measurement to discriminate between the Kondo breakdown and spin-density wave theories.

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Heavy-fermion quantum criticality is a typical example of a quantum system where both strong correlations and Fermi surface effects play a major role [1]. The standard model of quantum criticality in a metallic system is a $z = 2$ critical theory, often referred as Hertz-Moriya-Millis theory [2], where $z$ is the dynamical exponent relating the variation of the energy with the momentum, $\omega \sim q^z$. Unfortunately, many heavy fermion compounds have been shown not to follow the spin-density-wave (SDW) theoretical framework [3,4,5,6].

An interesting suggestion is that the heavy-fermion quantum transition is analogous to the Mott transition [7,8,9,10]. The arguments in support of this view are quantum transition is analogous to the Mott transition as an orbital selective Mott transition, where only the divergence of the effective mass near the QCP [5] and quantum criticality in a metallic system is a $z = 2$ critical theory, often referred as Hertz-Moriya-Millis theory [2], where $z$ is the dynamical exponent relating the variation of the energy with the momentum, $\omega \sim q^z$. Unfortunately, many heavy fermion compounds have been shown not to follow the spin-density-wave (SDW) theoretical framework [3,4,5,6].

Recently, this problem has been re-visited in the slave-boson context [9,10]. The main idea is that the Kondo breakdown QCP is multi-scale. Dynamics of hybridization (holon) fluctuations is governed by spinon-electron polarization. An important observation is that there should exist a Fermi surface mismatch $q^* = |k^f_F - k^c_F|$ between Fermi momentum $k^f_F$ for spinons and $k^c_F$ for conduction electrons since fillings of spinons and electrons differ from each other. Fermi surface mismatch gives rise to an energy gap $E^*$ for such spinon-electron fluctuations. Although it depends on the value of $q^*$, this energy scale is shown to vary from $O(10^0)$ mK to $O(10^5)$ mK. When $E < E^*$, holon fluctuations are undamped without considering gauge fluctuations, thus described by $z = 2$ dilute Bose gas model. On the other hand, when $E > E^*$, holon fluctuations are dissipative since spinon-electron excitations are Landau damped, thus described by $z = 3$ critical theory. Based on the $z = 3$ quantum criticality, recent studies [9,10] have found quasi-linear electrical transport and logarithmically divergent specific heat coefficient in $d = 3$, consistent with an experiment [6].

In this paper we study the Grüneisen ratio (GR) $\Gamma_s(r,T) \equiv \alpha_s(r,T)/c_s(r,T)$ based on the multi-scale Kondo breakdown QCP scenario [3,10], where $\alpha_s(r,T) = \frac{1}{T^4} \frac{\partial^2 \ln (r \gamma T)}{\partial T^2}$ and $c_s(r,T) = -T \frac{\partial^2 \ln r \gamma T}{\partial T^2}$ are thermal expansion and molar specific heat with molar volume $v$, respectively. Recently, GR has been proposed as one possible measure characterizing the nature of a QCP [11]. A remarkable feature is that the GR diverges at any QCP with an anomalous exponent depending on the nature of the quantum transition. Consider the scaling expression $f_s(r,T) = b^{-(d+z)} f_c(r \gamma T/b^d)$ for the free energy near a QCP at spacial dimension $d$, where $r \approx P_{P_0}$ is a distance from the QCP ($P_c$) with a pressure-unit constant $P_0$ and $b$ is a scaling parameter with a correlation-length exponent $\nu$. Evaluating the thermal expansion and molar specific heat, we find the following scaling expressions:

$$\Gamma_s(r,T = 0) = -G_P [v(P - P_e)]^{-1},$$

with $G_P = \nu (d-y_0) / y_0$ where $y_0$ is an exponent associated with the third law of thermodynamics [11], and

$$\Gamma_s(T; r = 0) = -G_T T^{-\nu z},$$

with $G_T = \frac{1}{T} \frac{\partial (\ln \gamma T)}{\partial (d+z)} - \frac{1}{P_0} \frac{\partial (\ln \gamma T)}{\partial P_0}$. The GR at the QCP, $\Gamma_s(T; r = 0)$ exhibits the scaling exponent $x = \frac{1}{\nu z}$ in any dimension.

In a recent measurement [12] it was reported that for $YbRh_2(Si_{0.95}Gd_{0.05})_2$, the specific heat coefficient can be well fitted by $\gamma(T) = C(T)/T \times \ln (T_P / T)$ for $0.3K < T < 10K$, with an energy scale $T_\gamma \approx 30K$ identified with its Kondo temperature, and $\gamma(T) \propto T^{-1/3}$ for $T \approx 0.3K$. The thermal expansion coefficient was fitted as (3) for $1K < T < 10K$ with a temperature scale $T_0 \approx 13K$, and $\alpha(T)/T \propto a_0 + a_1/T$ for $0.1K < T < 1K$ with $a_0 \approx 3.4 \times 10^{-6}K^{-2}$ and $a_1 \approx 1.34 \times 10^{-6}K^{-1}$. Finally, the experiment shows that the GR diverges with an exponent $x \approx 0.7 \pm 0.1$. This invalidates the SDW scenario, since we have $x = 1$ owing to $z = 2$ and $\nu = 1/2$, where this critical theory is beyond its upper critical dimension in $d \geq 2$.

In this study we show that the scenario of multi-scale Kondo breakdown QCP gives rise to a divergent GR with
the exponent 0.7. In particular, we fit the experimental data of YbRh$_2$(Si$_{0.95}$Ge$_{0.05}$)$_2$ for specific heat, thermal expansion, and GR with simple analytic expressions [Eqs. (3) and (4)], for which the asymptotic behavior is summarized in Table I. The $z = 3$ quantum criticality in $d = 3$ turns out to play an essential role for thermodynamics near the QCP of YbRh$_2$(Si$_{0.95}$Ge$_{0.05}$)$_2$.

$$\frac{\alpha_s(T)}{T^{1/3}} \sim -\frac{c_s(T)}{T \ln T} \sim -\frac{\Gamma_s(T)}{T^{-2/3}/\ln T}$$

TABLE I: Thermodynamics in the $z = 3$ regime ($d = 3$)

Interestingly, varying an external parameter gives an opportunity to distinguish the Kondo breakdown from the SDW scenario (see Fig. 1). It has been shown that the thermal expansion coefficient should change sign across the SDW QCP in the zero temperature limit, and GR also does accordingly [11]. In the Kondo breakdown scenario two kinds of collective excitations, hybridization and gauge fluctuations, contribute to thermal expansion. Hybridization fluctuations give rise to the same sign change as the SDW fluctuations while gauge fluctuations do not. Considering that gauge fluctuations should remain gapless in the spin liquid phase due to gauge invariance, their contribution for thermal expansion is vanishingly small in the spin liquid phase. On the other hand, they contribute to thermal expansion heavily, approaching the QCP in the heavy-fermion phase owing to the Anderson-Higgs mechanism. Taking into account both hybridization and gauge fluctuations, an asymmetric feature of GR is expected to appear around the Kondo breakdown QCP.

We start from the U(1) slave-boson representation of the Anderson lattice model in the large-$U$ limit

$$L = \sum_i c_{i\sigma}^\dagger (\partial_\tau - \mu)c_{i\sigma} - t \sum_{\langle ij \rangle} (c_{i\sigma}^\dagger c_{j\sigma} + H.c.)$$

$$+ V \sum_i (b_i f_{i\sigma}^\dagger c_{i\sigma} + H.c.) + \sum_i b_i^\dagger \partial_\tau b_i$$

$$+ \sum_i f_{i\sigma}^\dagger (\partial_\tau + \epsilon_f) f_{i\sigma} + \frac{J}{N} \sum_{\langle ij \rangle} (f_{i\sigma}^\dagger \chi_{ij} f_{j\sigma} + H.c.)$$

$$+ \sum_i \lambda_i (b_i^\dagger b_i + f_{i\sigma}^\dagger f_{i\sigma} - 1) + \frac{J}{N} \sum_{\langle ij \rangle} |\chi_{ij}|^2$$

Here, $c_{i\sigma}$ and $d_{i\sigma} = b_i^\dagger f_{i\sigma}$ are conduction electron with a chemical potential $\mu$ and localized electron with an energy level $\epsilon_f$ respectively, where $b_i$ and $f_{i\sigma}$ are holon and spinon, associated with hybridization and spin fluctuations. The spin-exchange term for the localized orbital is introduced for competition with the hybridization term, and decomposed via exchange hopping processes of spinons, where $\chi_{ij}$ is a hopping parameter for the decomposition. $\lambda_i$ is a Lagrange multiplier field to impose the single occupancy constraint $b_i^\dagger b_i + f_{i\sigma}^\dagger f_{i\sigma} = N/2$, where $N$ is the number of fermion flavors with $\sigma = 1, ..., N$.

The slave-boson mean-field analysis has shown an orbital selective Mott transition [12] as breakdown of Kondo effect at $J \approx T_K$, where $T_K = D \exp(\frac{\mu_e}{\epsilon_f})$ is the Kondo temperature with the density of states $\rho_e$ for conduction electrons [8]. If we try to understand the GR in this level of approximation, we find $x = 1$ for the GR exponent. Actually, one can check that the mean-field free energy satisfies the following scaling behavior $f_{MF}(B, T) = T^{\frac{1}{\gamma_{MF}}} F( BT^{-\gamma_{MF}} )$, where $F(x)$ is an analytic function and $B = V(b)$ is the effective hybridization.

Fluctuation-corrections are important at the Kondo breakdown QCP, where both hybridization and gauge fluctuations should be taken into account carefully. Such fluctuations are treated on an equal footing in the Eliashberg framework, where momentum dependence in self-energies and vertex corrections are neglected, justified by the Migdal theorem and large $N$ approximation [9, 10].

For a systematic study of thermodynamics, we construct a Luttinger-Ward (LW) functional in the Eliashberg framework, composed of contributions from conduction electrons, spinons, holons, gauge fluctuations and their self-energy parts. One can derive self-consistent Eliashberg equations for the self-energies from variation of the LW functional with respect to each self-energy. Using these equations, one is allowed to simplify the LW functional as $F_{LW} = F_{FL} + F_{FL}^t + F_b + F_{\sigma}$, where the first two parts represent Fermi liquid contributions for conduction electrons and spinons while the latter two parts express hybridization and gauge contributions, respectively. Such fermion contributions are sub-dominant compared with boson contributions, and they can be ig-
nored in the low energy limit. Accordingly, thermal expansion and specific heat can be approximated as follows near the Kondo breakdown QCP, $\alpha_s(T) \approx \alpha_b(T) + \alpha_a(T)$ and $c_s(T) \approx c_b(T) + c_a(T)$, respectively. As a result, the GR is found to be $\Gamma_s(T) \approx \alpha_b(T) + \alpha_a(T) / c_b(T) + c_a(T)$.

The bosonic part of the free energy is given by

$$F_s(T) = T \sum_{\Delta} \int \frac{q^3 dq}{(2\pi)^3} \ln\left(q^2 + \frac{[\Omega(b)]^2}{q} + 2\Delta_b\right)$$

$$+ T \sum_{\Delta} \int \frac{q^3 dq}{(2\pi)^3} \ln\left(q^2 + \frac{[\Omega(a)]^2}{q} + \Delta_a\right) + F_s(2)$$

Here, $\gamma_b = \frac{2\pi}{\alpha_F}$ and $\gamma_a = \frac{3\pi}{\alpha_F} + \frac{3\pi v_F^2 \rho_c}{4\alpha u_b}$ are Landau damping coefficients for holon and gauge fluctuations, respectively, where $v_F$ is the Fermi velocity for conduction electrons, $\alpha = \frac{1}{\alpha_F}$ is an effective ratio between bandwidth of each fermion sector, and $f_d$ is associated with an ultra-violet cutoff for gauge fluctuations. $\Delta_b$ is the mass for the hybridization fluctuations, identifying the Kondo breakdown QCP with $\Delta_b = 0$. $\Delta_a$ is the mass for gauge fluctuations, resulting from Anderson-Higgs mechanism, thus related with the mass of holon as $\Delta_a = \frac{3N V^4 \rho_c^2}{4\alpha u_b} \Delta_b$, where $u_b$ is the strength of local interactions for holons, phenomenologically introduced. $F_c$ is the condensation part.

Performing the frequency summation and momentum integral, we find the specific heat and thermal expansion coefficients at the QCP,

$$c_s(T > E^*) \frac{T}{c_s} = C_c \left\{ \gamma_b \ln \left( \frac{A}{E} \right) + \gamma_a \ln \left( \frac{\gamma_a}{\gamma_a T} \right) \right\},$$

$$c_s(T < E^*) \frac{T}{c_s} = C_c \left\{ \gamma_b \ln \left( \frac{A}{E} \right) + \gamma_a \ln \left( \frac{\gamma_a}{\gamma_a T} \right) \right\}$$

(3)

and

$$\alpha_s(T > E^*) \frac{T}{\alpha_s} = C_c \frac{\partial \Delta_b}{\partial P} \left( 2\gamma_b^* + \frac{3N V^4 \rho_c^2}{4\alpha u_b} \gamma_b^* \right) T^{-\frac{4}{3}},$$

$$\alpha_s(T < E^*) \frac{T}{\alpha_s} = C_c \frac{\partial \Delta_a}{\partial P} \left( 2\gamma_a^* + \frac{3N V^4 \rho_c^2}{4\alpha u_b} \gamma_a^* T^{-\frac{4}{3}} \right),$$

(4)

where $C_c = \frac{4}{3\pi} J_0^\infty dy \left( -\frac{y^2}{\sinh^2 y} + \frac{y^3 \coth y}{\sinh^2 y} \right)$ and $C_c = \frac{4}{\pi} \left( J_0^\infty dx \frac{x^3}{1+e^{-x}} \right) \left( J_0^\infty dy \frac{y^2}{\sinh y} \right)$ are positive numerical constants. The condensation part is assumed to be almost constant for temperature dependence, thus can be ignored for thermal expansion. Note that there is an unknown constant $\frac{\partial \Delta}{\partial P}$ with pressure $P$ in the thermal expansion coefficient, determining its overall sign. Recalling that it is negative for $YbRh_2\{Si_{0.95}Ge_{0.05}\}$ [12], we see $\frac{\partial \Delta_b}{\partial P} < 0$. This implies that pressure puts the QCP of $YbRh_2\{Si_{0.95}Ge_{0.05}\}$ toward the heavy-fermion side if it is identified with the Kondo breakdown QCP. One can check that holon thermodynamics is consistent with $z = 3$ scaling for $T > E^*$ while gauge thermodynamics is for all temperatures. In addition, both specific heat and thermal expansion coefficients are constant for holon fluctuations at $T < E^*$, consistent with Fermi liquid physics.

Using Eqs. (3) and (4), we try to fit the experimental data of Ref. [12]. The density of states $\rho_c = \frac{\pi}{k_F}$ for conduction electron with the bandwidth $D = 6t = 10^4 K$ and the ratio between bandwidths $\alpha = 10^{-3}$ are fixed. Considering $v_F = \frac{k_F}{\mu^2} \approx 2t$ for the sphere Fermi surface, $\gamma_b$ is determined as $\gamma_b = 2.693$. $V$ can be deduced from the Kondo temperature $T_K \approx 30 K$ with $\epsilon_f = -\frac{D}{2}$, thus $V = 0.293 D$. $f_d$ is used as a fitting parameter, determining $\gamma_a = 1.367$. The cutoff $\Lambda$ in specific heat is set to be an effective bandwidth for localized spins, i.e., $\Lambda \approx \alpha D$. $E^*$ is approximately given by the upturn temperature for
specific heat, here $E^* \approx 0.3K$. For thermal expansion, we have two free parameters, $u_b$ and $\Delta u_b^2$.

Fig. 2 shows the fitting for the specific heat coefficient $c_s(T)/T$. For $T > E^*$, we have a very good matching unlike for $T < E^*$. Although the origin of this upturn behavior is not explained yet clearly, two dimensional ferromagnetic fluctuations may give one possible explanation, resulting in $c_s(T)/T \propto T^{-1/3}$. From the inset figure, we can conclude that both hybridization and gauge fluctuations are important for specific heat near the Kondo breakdown QCP. Considering that the hybridization fluctuations arise from collective excitations of conduction electrons and spinons, and gauge fluctuations result from spinon current-current correlations, one can expect that both fluctuations will contribute in a similar fashion.

Fig. 3 shows the fitting for the thermal expansion coefficient $C_0(T)/T$, where we have a rather good agreement between experiment and theory. Although we have used two free parameters $u_b$ and $\Delta u_b^2$, such parameters can change only the overall scale, thus one may regard that only one parameter is used. The inset figure exhibits that contributions from gauge fluctuations are much larger than those from hybridization ones. Although this physics depends on the local-interaction strength $u_b$ for hybridization fluctuations, it is valid as far as $u_b \ll \frac{1}{D \alpha}$ is satisfied in Eq. (4), i.e., in the weak coupling limit preserving the present picture of the Kondo breakdown QCP. Our fitting for the thermal expansion coefficient may be the first explicit demonstration, supporting importance of gauge fluctuations.

In conclusion, we have fitted the experimental data of $YbRh_2(Sc_{0.35}Ge_{0.65})_2$ for specific heat, thermal expansion and Gr"uneisen ratio based on simple analytic formulae in the multi-scale Kondo breakdown scenario. Both hybridization and gauge fluctuations contribute to specific heat in a similar fashion around the QCP. Gauge fluctuations are more important in the heavy-fermion phase than in the spin liquid phase for thermal expansion, causing an asymmetry for Gr"uneisen ratio around the QCP. This feature can be used to discriminating the Kondo breakdown scenario from the SDW framework. These $z = 3$ critical fluctuations explain the divergent Gr"uneisen ratio with the anomalous exponent 0.7 beyond the SDW theory. We suggest that two dimensional ferromagnetic fluctuations may give one possible explanation for thermodynamics in the low temperature region below $E^*$, not captured in the present framework.

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