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Quantum Valence Criticality as an Origin of Unconventional Critical Phenomena

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It is shown that unconventional critical phenomena commonly observed in paramagnetic metals YbRh_2Si_2 , $\text{YbRh}_2(\text{Si}_{0.95}\text{Ge}_{0.05})_2$, and $\beta\text{-YbAlB}_4$ are naturally explained by the quantum criticality of Yb-valence fluctuations. We construct the mode-coupling theory taking account of local correlation effects of f electrons and find that unconventional criticality is caused by the locality of the valence fluctuation mode. We show that measured low-temperature anomalies such as divergence of uniform spin susceptibility $\chi \sim T^{-\zeta}$ with $\zeta \sim 0.6$ giving rise to a huge enhancement of the Wilson ratio and the emergence of T -linear resistivity are explained in a unified way.

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Anomalous critical phenomena, which do not follow the conventional spin-fluctuation theories [1–4] have been discovered in paramagnetic metal phases in YbRh_2Si_2 [5,6], $\text{YbRh}_2(\text{Si}_{0.95}\text{Ge}_{0.05})_2$ [7,8], and $\beta\text{-YbAlB}_4$ [9]. The most striking anomaly is that low-temperature uniform spin susceptibility exhibits divergent behavior $\chi(T) \sim T^{-\zeta}$ with the anomalous critical exponent $\zeta = 0.6$ in $\text{YbRh}_2(\text{Si}_{0.95}\text{Ge}_{0.05})_2$ and $\zeta = 0.5$ in $\beta\text{-YbAlB}_4$ in spite of no sign of a ferromagnetic phase nearby. In these materials, the Sommerfeld constant exhibits the logarithmic divergence $\gamma_e = C_e/T \sim -\ln T$ [5,8,9], giving rise to a large Wilson ratio, i.e., a dimensionless ratio of χ to γ_e , $R_W = 17.5$ in $\text{YbRh}_2(\text{Si}_{0.95}\text{Ge}_{0.05})_2$ [7], and $R_W = 6.5$ in $\beta\text{-YbAlB}_4$ [9], exceeding the conventional strong-coupling value $R_W = 2$. The linear- T dependence of low- T resistivity emerges in a wide- T range in YbRh_2Si_2 [5], $\text{YbRh}_2(\text{Si}_{0.95}\text{Ge}_{0.05})_2$ [8], and also $\beta\text{-YbAlB}_4$ [9]. These observations suggest that there exists a new class of materials showing similar critical phenomena, which are unconventional.

So far, to explain YbRh_2Si_2 and $\text{YbRh}_2(\text{Si}_{0.95}\text{Ge}_{0.05})_2$, theoretical efforts have been made [10–12]. In particular, a scenario asserting that f electrons undergo a localized to itinerant transition was extensively discussed [10,11]. However, YbRh_2Si_2 shows a large Sommerfeld constant as $\sim 1.7/\text{J mol K}^2$ even inside of the antiferromagnetic (AF) phase [8], indicating that heavy quasiparticles are responsible for the AF state. Indeed, a band-structure calculation showed evidence contrary to the scenario [13] by demonstrating that a tiny valence change of Yb can explain the Hall-coefficient measurement in YbRh_2Si_2 [14].

Recently, in $\beta\text{-YbAlB}_4$ the valence of Yb has been detected as $\text{Yb}^{+2.75}$ (0.75 $4f$ hole per Yb) at $T = 20$ K, suggesting strong valence fluctuations [15]. Close relation of anomalous critical phenomena and valence fluctuations has been also indicated in $\text{Ce}_{0.9-x}\text{Th}_{0.1}\text{La}_x$ [16] and in YbAuCu_4 [17]. Both are related to typical

valence-transition materials: One is Ce metal, well known as $\gamma - \alpha$ transition [18], and the other is YbInCu_4 [19], both showing a discontinuous valence jump of a Ce and Yb ion, respectively, when T and P are varied. Since the first-order valence transition is an isostructural transition, the critical end point exists in the T - P (and chemical composition) phase diagram, as in the liquid-gas transition.

At $x \approx 0.1$ in $\text{Ce}_{0.9-x}\text{Th}_{0.1}\text{La}_x$, at which the critical end point is most suppressed and is close to $T = 0$ K [16], critical phenomena rising from the quantum critical end point were revealed: T -linear resistivity emerges prominently and uniform spin susceptibility is enhanced at low T giving rise to a large Wilson ratio, $R_W \sim 3$. In YbAuCu_4 , the uniform spin susceptibility is enhanced as $\chi(T) \sim T^{-0.6}$ as T decreases in spite of the fact that the AF transition takes place at $T_N = 0.8$ K [20], similarly to YbRh_2Si_2 . Furthermore, the sharp Yb-valence crossover temperature $T_v^*(H)$ is induced by applying a magnetic field [17], suggesting that YbAuCu_4 is located in the vicinity of the quantum critical end point of the valence transition. It should also be noted that the T - H phase diagram of YbAuCu_4 [17] closely resembles that of YbRh_2Si_2 [6]. The H dependence of the crossover temperature $T^*(H)$, emerging in several physical quantities [6], whose origin is unclear in YbRh_2Si_2 is quite similar to the $T_v^*(H)$ in YbAuCu_4 .

These observations strongly suggest the importance of quantum criticality of valence transition as a key mechanism of unconventional critical phenomena. From this viewpoint, in this Letter, we resolve this outstanding puzzle by showing that (a) uniform spin susceptibility diverges with anomalous criticality $\chi(T) \sim T^{-\zeta}$ with $0.5 \leq \zeta \leq 0.7$ in paramagnetic metals even without proximity to a ferromagnetic phase and (b) T -linear resistivity emerges in the wide- T range.

Let us start our discussion by introducing a minimal model which describes the essential part of the Ce- and Yb-based systems in the standard notation: $H = H_c + H_f + H_{\text{hyb}} + H_{U_{fc}}$, where $H_c = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma}$,

$H_f = \varepsilon_f \sum_{i\sigma} n_{i\sigma}^f + U_{ff} \sum_{i=1}^N n_{i\uparrow}^f n_{i\downarrow}^f$, $H_{\text{hyb}} = \sum_{\mathbf{k}\sigma} V_{\mathbf{k}} (f_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + c_{\mathbf{k}\sigma}^\dagger f_{\mathbf{k}\sigma})$, and $H_{U_{fc}} = U_{fc} \sum_{i=1}^N n_i^f n_i^c$. The U_{fc} term is the Coulomb repulsion between $4f$ and conduction electrons (holes) in Ce (Yb) systems, which is considered to play an important role in the valence transition [21].

To consider correlation effects by U_{ff} , we employ the slave-boson large- N expansion framework [22]. The Hamiltonian H is generalized to the case with N -fold degeneracy from $\sigma = \uparrow, \downarrow$, and the slave-boson operator b_i is introduced to eliminate the doubly-occupied state for $U_{ff} \rightarrow \infty$ under the constraint $\sum_m n_{im}^f + N b_i^\dagger b_i = 1$. The Lagrangian is written as $\mathcal{L} = \mathcal{L}_0 + \mathcal{L}'$:

$$\begin{aligned} \mathcal{L}_0 &= \sum_{\mathbf{k}m} c_{\mathbf{k}m}^\dagger (\partial_\tau + \bar{\varepsilon}_{\mathbf{k}}) c_{\mathbf{k}m} + \sum_{\mathbf{k}\mathbf{k}'} f_{\mathbf{k}m}^\dagger (\partial_\tau + \bar{\varepsilon}_{\mathbf{k}-\mathbf{k}'}^f) f_{\mathbf{k}'m} \\ &\quad + \frac{V}{\sqrt{N_s}} \sum_{\mathbf{k}\mathbf{k}'} (c_{\mathbf{k}m}^\dagger f_{\mathbf{k}'m} b_{\mathbf{k}-\mathbf{k}'}^\dagger + \text{H.c.}) + \frac{N}{N_s} \sum_{\mathbf{k}\mathbf{k}'} b_{\mathbf{k}}^\dagger \lambda_{\mathbf{k}-\mathbf{k}'} b_{\mathbf{k}'} \\ \mathcal{L}' &= -\frac{U_{fc}}{2} \sum_{im} (n_{im}^c + n_{im}^f) + \frac{U_{fc}}{N} \sum_{imm'} n_{im}^f n_{im'}^c, \end{aligned}$$

where $\lambda_{\mathbf{k}}$ is the Lagrange multiplier to impose the constraint, and $\bar{\varepsilon}_{\mathbf{k}} \equiv \varepsilon_{\mathbf{k}} + \frac{U_{fc}}{2}$ and $\bar{\varepsilon}_{\mathbf{k}-\mathbf{k}'}^f \equiv (\varepsilon_f + \frac{U_{fc}}{2}) \delta_{\mathbf{k}\mathbf{k}'} + \frac{1}{\sqrt{N_s}} \lambda_{\mathbf{k}-\mathbf{k}'}$. We here separate \mathcal{L} as \mathcal{L}_0 and \mathcal{L}' to perform the expansion with respect to the U_{fc} term after taking account of the local correlation of the U_{ff} term.

For $\exp(-S_0)$ with the action $S_0 = \int_0^\beta d\tau \mathcal{L}_0(\tau)$, the saddle point solution is obtained via the stationary condition $\delta S_0 = 0$ by approximating spatially uniform and time independent ones, i.e., $\lambda_{\mathbf{q}} = \lambda \delta_{\mathbf{q}}$ and $b_{\mathbf{q}} = b \delta_{\mathbf{q}}$. The solution is obtained by solving mean-field equations $\partial S_0 / \partial \lambda = 0$ and $\partial S_0 / \partial b = 0$ self-consistently.

For $S' = \int_0^\beta d\tau \mathcal{L}'(\tau)$, we introduce the identity applied by a Stratonovich-Hubbard transformation $e^{-S'} = \int \mathcal{D}\varphi \exp[\sum_{im} \int_0^\beta d\tau \{-\frac{U_{fc}}{2} \varphi_{im}(\tau)^2 + i \frac{U_{fc}}{\sqrt{N}} (c_{im} f_{im}^\dagger - f_{im} c_{im}^\dagger) \varphi_{im}(\tau)\}]$. The partition function is expressed as $Z = \int \mathcal{D}(c c^\dagger f f^\dagger) \exp(-S)$ with $S = S_0 + S'$. By performing Grassmann number integrations for $c c^\dagger$ and $f f^\dagger$, we obtain $Z = \int \mathcal{D}\varphi \exp(-S[\varphi])$ with $S[\varphi] = \sum_m \sum_{\bar{q}} \varphi_m(\bar{q}) \varphi_m(-\bar{q}) - \text{Tr} \ln[-\hat{G}_0^{-1} + \hat{V}] - \frac{\beta N}{\sqrt{N_s}} \lambda |b|^2 + \beta N q_0 \sqrt{N_s} \lambda$. Here, the abbreviation $\bar{q} \equiv (\mathbf{q}, i\omega_l)$ with $\omega_l = 2l\pi T$ is used, and \hat{G}_0 and \hat{V} are defined as

$$\hat{G}_0^{-1} \equiv \begin{pmatrix} i\varepsilon_n - \bar{\varepsilon}_{\mathbf{k}} & -\frac{Vb^*}{\sqrt{N_s}} \\ -\frac{Vb}{\sqrt{N_s}} & i\varepsilon_n - \bar{\varepsilon}_0^f \end{pmatrix} \delta_{\mathbf{k}\mathbf{k}'}, \quad \hat{V} \equiv \begin{pmatrix} 0 & \tilde{\varphi}_{m\bar{k}\bar{k}'} \\ \tilde{\varphi}_{m\bar{k}\bar{k}'} & 0 \end{pmatrix}$$

with $\tilde{\varphi}_{m\bar{k}\bar{k}'} \equiv \frac{U_{fc}}{\sqrt{\beta N N_s}} \varphi_m(\bar{k} - \bar{k}')$, respectively. Here, $\bar{k} \equiv (\mathbf{k}, i\varepsilon_n)$ with $\varepsilon_n = (2n+1)\pi T$, and each matrix element of \hat{G}_0 is defined as $(\hat{G}_0)_{11} \equiv G_0^{cc}$, $(\hat{G}_0)_{12} \equiv G_0^{cf}$, $(\hat{G}_0)_{21} \equiv G_0^{fc}$,

and $(\hat{G}_0)_{22} \equiv G_0^{ff}$. By using $\text{Tr} \ln[-\hat{G}_0^{-1} + \hat{V}] = \text{Tr} \ln[-\hat{G}_0^{-1}] - \sum_{n=1}^\infty \frac{1}{n} \text{Tr}(\hat{G}_0 \hat{V})^n$, we obtain

$$\begin{aligned} S[\varphi] &= \sum_m \left[\frac{1}{2} \sum_{\bar{q}} \Omega_2(\bar{q}) \varphi_m(\bar{q}) \varphi_m(-\bar{q}) + \sum_{\bar{q}_1, \bar{q}_2, \bar{q}_3} \Omega_3(\bar{q}_1, \bar{q}_2, \bar{q}_3) \right. \\ &\quad \times \varphi_m(\bar{q}_1) \varphi_m(\bar{q}_2) \varphi_m(\bar{q}_3) \delta\left(\sum_{i=1}^3 \bar{q}_i\right) \\ &\quad + \sum_{\bar{q}_1, \bar{q}_2, \bar{q}_3, \bar{q}_4} \Omega_4(\bar{q}_1, \bar{q}_2, \bar{q}_3, \bar{q}_4) \times \varphi_m(\bar{q}_1) \varphi_m(\bar{q}_2) \\ &\quad \times \varphi_m(\bar{q}_3) \varphi_m(\bar{q}_4) \delta\left(\sum_{i=1}^4 \bar{q}_i\right) + \cdots \left. \right]. \end{aligned} \quad (2)$$

Here, constant terms independent of $\varphi_m(\bar{q})$ are omitted in Eq. (2) since they merely shift the origin of the free energy of the system. The coefficient of the quadratic term is given by

$$\Omega_2(\mathbf{q}, i\omega_l) = U_{fc} \left[1 - \frac{2U_{fc}}{N} \{ \chi_0^{ffcc}(\mathbf{q}, i\omega_l) - \chi_0^{cfcf}(\mathbf{q}, i\omega_l) \} \right], \quad (3)$$

where $\chi_0^{\alpha\beta\gamma\delta}(\mathbf{q}, i\omega_l) \equiv -\frac{T}{N_s} \sum_{\mathbf{k}, n} G_0^{\alpha\beta}(\mathbf{k} + \mathbf{q}, i\varepsilon_n + i\omega_l) G_0^{\gamma\delta}(\mathbf{k}, i\varepsilon_n)$. Since long wavelength $|\mathbf{q}| \ll q_c$ around $\mathbf{q} = \mathbf{0}$ and low frequency $|\omega| \ll \omega_c$ regions play dominant roles in critical phenomena with q_c and ω_c being cutoffs for momentum and frequency in the order of inverse of the lattice constant and the effective Fermi energy, respectively, Ω_i for $i = 2, 3$, and 4 are expanded for q and ω around $(\mathbf{0}, 0)$:

$$\Omega_2(\mathbf{q}, i\omega_l) \approx \eta + Aq^2 + C \frac{|\omega_l|}{q} \quad (4)$$

where $\eta = U_{fc} [1 - \frac{2U_{fc}}{N} \{ \chi_0^{ffcc}(\mathbf{0}, 0) - \chi_0^{cfcf}(\mathbf{0}, 0) \}]$, $\Omega_3(q_1, q_2, q_3) \approx v_3 / \sqrt{\beta N_s}$, and $\Omega_4(q_1, q_2, q_3, q_4) \approx v_4 / (\beta N_s)$.

Different from ordinary critical phenomena of spin fluctuations [1–4], there appears a cubic term in Eq. (2) in general for the valence fluctuation case [23]. Let us here apply the Hertz's renormalization-group procedure [3] to $S[\varphi]$: (a) Integrating out high momentum and frequency parts for $q_c/s < q < q_c$ and $\omega_c/s^z < \omega < \omega_c$, respectively, with s being a dimensionless scaling parameter ($s \geq 1$) and z the dynamical exponent. (b) Scaling of q and ω by $q' = sq$ and $\omega' = s^z \omega$. (c) Rescaling of φ by $\varphi'(\mathbf{q}', \omega') = s^a \varphi(\mathbf{q}/s, \omega'/s)$. Then, we determined that to make the Gaussian term in Eq. (2) scale invariant, a must satisfy $a = -(d+z+2)/2$ with d spatial dimension and the dynamical exponent $z = 3$. The renormalization-group equations for coupling constants v_j are derived as $\frac{dv_3}{ds} = [6 - (d+z)]v_3 + O(v_3^2)$, and $\frac{dv_4}{ds} = [4 - (d+z)]v_4 + O(v_4^2)$, for cubic and quadratic terms, respectively. By solving these equations, it is shown that higher order terms than the Gaussian term are irrelevant

$$\lim_{s \rightarrow \infty} v_j(s) = 0 \quad \text{for } j \geq 3 \quad (5)$$

for $d + z > 6$. For the case of $d = 3$ and $z = 3$, it is shown that the cubic term is marginally irrelevant [21]. Hence, the universality class of the criticality of valence fluctuations belongs to the Gaussian fixed point. This implies that critical valence fluctuations are qualitatively described by the RPA framework with respect to U_{fc} . The coefficient of the Gaussian term in Eq. (2) is nothing but the inverse of the valence susceptibility $\Omega_2(\mathbf{q}, i\omega_l) \equiv \chi_v(\mathbf{q}, i\omega_l)^{-1}$. Since evaluation of $\chi_0^{ffcc}(\mathbf{q}, i\omega_l)$ and $\chi_0^{cfcf}(\mathbf{q}, i\omega_l)$ using the saddle point solution for $\exp(-S_0)$ concludes $\chi_0^{ffcc} \gg \chi_0^{cfcf}$ (see Fig. 2 and text below), it turns out that χ_v is expressed by the RPA form $\chi_v(\mathbf{q}, i\omega_l) = \int_0^\beta d\tau \langle T_\tau n_f(\mathbf{q}, \tau) n_f(-\mathbf{q}, 0) \rangle e^{i\omega_l \tau} \approx U_{fc}^{-1} [1 - \frac{2U_{fc}}{N} \chi_0^{ffcc}(\mathbf{q}, i\omega_l)]^{-1}$, as shown in Fig. 1.

An important consequence of this result is that dynamical f -spin susceptibility $\chi_f^{+-}(\mathbf{q}, i\omega_l) \equiv \int_0^\beta d\tau \langle T_\tau S_f^+(\mathbf{q}, \tau) S_f^-(\mathbf{q}, 0) \rangle e^{i\omega_l \tau}$ has a common structure with χ_v in the RPA framework as shown in Fig. 1. At the quantum critical end point of the valence transition, namely, the quantum critical point (QCP), the valence susceptibility $\chi_v(\mathbf{0}, 0)$ diverges. The common structure indicates that $\chi_f^{+-}(\mathbf{0}, 0)$ also diverges at the QCP. The uniform spin susceptibility is given by $\chi \approx \chi_s^f \approx \frac{3}{2} \mu_B^2 g_f^2 \chi_f^{+-}(\mathbf{0}, 0)$ with χ_s^f uniform f -spin susceptibility, μ_B the Bohr magneton, and g_f Lande's g factor for f electrons. This gives a qualitative explanation for the fact that uniform spin susceptibility diverges at the QCP of valence transition under a magnetic field, which was shown by the slave-boson mean-field theory applied to the Hamiltonian H [24]. Numerical calculations for H in $d = 1$ by the density matrix renormalization group [24] and in $d = \infty$ by the dynamical mean field theory [25] also showed the simultaneous divergence of χ_v and uniform spin susceptibility under the magnetic field, reinforcing the above argument based on RPA.

The other important point of the present theory is that the “unperturbed” term \mathcal{L}_0 , i.e., \hat{G}_0 , already contains the local correlation effect by U_{ff} . This effect plays a key role in critical phenomena in Ce- and Yb-based systems, which will be shown below to be the origin of the unconventional criticality. The local correlation effect emerges as dispersionless, almost q -independent $\chi_0^{ffcc}(\mathbf{q}, 0)$ and $\chi_0^{cfcf}(\mathbf{q}, 0)$ in Eq. (3), as shown in Fig. 2(a). Here, the saddle point solution for $\exp(-S_0)$ is employed for a typical parameter set of heavy-electron systems: $D = 1$, $V = 0.5$, and $U_{ff} = \infty$ at total filling $n = 7/8$ with

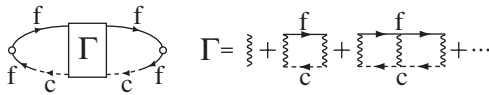


FIG. 1. Feynman diagrams for dynamical valence susceptibility and dynamical spin susceptibility for f electrons. Solid lines and dashed lines represent the f - and conduction-electron Green functions, G_0^{ff} and G_0^{cc} , respectively. Wiggly lines represent U_{fc} .

$\varepsilon_{\mathbf{k}} = \mathbf{k}^2/(2m_0) - D$ and $n \equiv \bar{n}_f + \bar{n}_c$, where \bar{n}_f and \bar{n}_c are the number of f electrons and conduction electrons per “spin” and site, respectively. The bare mass m_0 is chosen such that the integration from $-D$ to D of the density of states of conduction electrons per “spin” is equal to 1. This local nature is reflected in the inverse of valence susceptibility in Eq. (4) as an extremely small coefficient A . We note here that this flat- q result is obtained not only for deep ε_f with $\bar{n}_f = 1/2$ in the Kondo regime, but also for shallow ε_f with $\bar{n}_f < 1/2$ in the valence-fluctuating regime [see Fig. 2(b)]. Here, we note that the $c - f$ hybridization is always finite.

To clarify how this local nature causes unconventional criticality, we construct a self-consistent renormalization (SCR) theory for valence fluctuations. Although higher order terms v_j ($j \geq 3$) in $S[\varphi]$ are irrelevant as shown in Eq. (5), the effect of their mode couplings affects low- T physical quantities significantly as is well known in spin-fluctuation theories [1–4]. To construct the action using the best Gaussian taking account of the mode-coupling effects up to the 4th order ($j \leq 4$) in $S[\varphi]$, we employ Feynman’s inequality on the free energy: $F \leq F_{\text{eff}} + T \langle S - S_{\text{eff}} \rangle_{\text{eff}} \equiv \tilde{F}(\eta)$. Here, $S_{\text{eff}}[\varphi] = \frac{1}{2} \sum_{\mathbf{m}} \sum_{\mathbf{q}, l} (\eta + Aq^2 + C_q |\omega_l|) |\varphi_{\mathbf{m}}(\mathbf{q}, i\omega_l)|^2$, and η is determined to make $\tilde{F}(\eta)$ be optimum. By optimal condition $d\tilde{F}(\eta)/d\eta = 0$, the self-consistent equation for η , i.e., the SCR equation, is obtained: $\eta = \eta_0 + 3v_4 \langle \varphi_m^2 \rangle_{\text{eff}}^2 / N_s$, where $\langle \varphi_m^2 \rangle_{\text{eff}} = T \sum_{\mathbf{q}, l} (\eta + Aq^2 + C_q |\omega_l|)^{-1}$. Here, we write $\langle \varphi_m^2 \rangle_{\text{eff}}$ in a general form using C_q , which is given by $C_q \equiv C / \max\{q, l_i^{-1}\}$ with l_i being the mean-free path by impurity scattering [26]. When the system is clean, i.e., $C_q = C/q$, the SCR equation in $d = 3$ in the $Aq_B^2 \lesssim \eta$ regime with q_B being the momentum at the Brillouin Zone is given by

$$y = y_0 + \frac{3}{2} y_1 t \left[\frac{x_c^3}{6y} - \frac{1}{2y} \int_0^{x_c} dx \frac{x^3}{x + \frac{t}{6y}} \right], \quad (6)$$

where $y \equiv \eta/(Aq_B^2)$, $t \equiv T/T_0$, $T_0 \equiv Aq_B^3/(2\pi C)$, $x \equiv q/q_B$, $x_c \equiv q_c/q_B$, and y_0 and y_1 are constants. When $y \gg t$, $y \propto t^{2/3}$ is obtained from Eq. (6) at the QCP with $y_0 = 0$. This indicates that the valence susceptibility

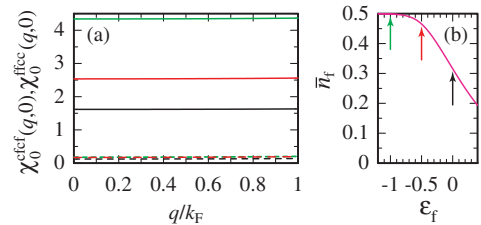


FIG. 2 (color). (a) q dependence of $\chi_0^{ffcc}(q, 0)$ (solid line) and $\chi_0^{cfcf}(q, 0)$ (dashed line) calculated by using saddle point solution of $\exp(-S_0)$ for $\varepsilon_f = -1$ (green), -0.5 (red), and 0.0 (black). (b) \bar{n}_f vs ε_f . (a) and (b) are results for $D = 1$, $V = 0.5$, and $U_{ff} = \infty$ at $n = 7/8$.

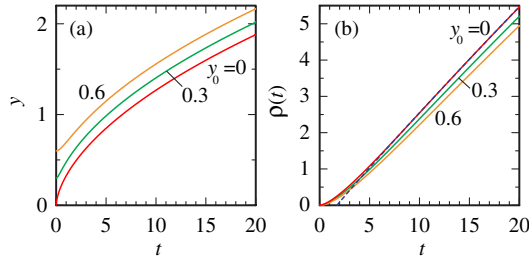


FIG. 3 (color online). (a) Numerical solutions of Eq. (6) for $y_0 = 0.0$ (at QCP), 0.3, and 0.6 at $y_1 = 1$ and $x_c = 1$. (b) Electrical resistivity $\rho(T)$ calculated by using $y(t)$ in (a). Dashed line represents the linear- t fit.

shows unconventional criticality $\chi_v(\mathbf{0}, 0) = \eta^{-1} \propto t^{-2/3}$. Figure 3(a) shows numerical solutions of Eq. (6). Note here that the coefficient A is quite small as shown above, giving rise to quite small $T_0 (= Aq_B^3/(2\pi C) \ll T_F)$ so that the region of $t \equiv T/T_0$ shown in Fig. 3 corresponds to that of $T \ll T_F \sim O(D)$. Hence, a wide range of $t = T/T_0$ is shown in the plot. The least square fit of the data for $5 \leq t \leq 100$ gives $y \propto t^{0.551}$. Since the Gaussian fixed point ensures the simultaneous divergence of valence susceptibility and uniform f -spin susceptibility as discussed above, χ_s^f shows divergent behavior $\sim t^{-\zeta}$ with $0.5 \leq \zeta \leq 0.7$ depending on the temperature range in agreement with experiments in $\text{YbRh}_2(\text{Si}_{0.95}\text{Ge}_{0.05})_2$ and $\beta\text{-YbAlB}_4$. We note that the NMR or NQR relaxation rate is shown to be $(T_1 T)^{-1} \sim \chi_s^f(t) \propto t^{-\zeta}$, which also quantitatively agrees with $(T_1 T)^{-1} \sim T^{-0.5}$ in YbRh_2Si_2 [27].

We should note here that in the $T \rightarrow 0$ limit, although it may be experimentally difficult to access such a low temperature overcoming the smallness of A , the SCR equation follows the conventional $z = 3$ type [1,3,4] in the clean system, giving rise to $y \propto t^{4/3}$. Then, at the QCP ($y_0 = 0$), as t decreases, a crossover from $y \propto t^{2/3}$ to $y \propto t^{4/3}$ occurs. In reality, however, because of the smallness of A , the low- T range is extremely elongated by the relation $t = T/T_0$ with $T_0 \propto A$, which makes it possible that unconventional criticality dominates over the experimentally accessible low-temperature region.

We note that the electrical resistivity $\rho(T)$ shows a T -linear dependence in the regime $t \gtrsim 5$ ($y \gtrsim 1$) where Eq. (6) is applicable, as shown in Fig. 3(b). Here, following a formalism of Ref. [28], $\rho(T)$ is calculated as $\rho(T) \propto \frac{1}{T} \int_{-\infty}^{\infty} d\omega \omega n(\omega) [n(\omega) + 1] \int_0^{q_c} dq q^3 \text{Im} \chi_v^R(q, \omega)$ with $n(\omega) = 1/(e^{\beta\omega} - 1)$ being the Bose distribution function, and $\chi_v^R(q, \omega) = (\eta + Aq^2 - iC_q\omega)^{-1}$, a retarded valence susceptibility. Here, $y(t)$ in Fig. 3(a) is used for the clean system $C_q = C/q$, and the normalization constant is taken as 1 in the $\rho(t)$ plot. The emergence of $\rho(t) \propto t$ behavior can be understood from the locality of valence fluctuations: In the system with a small coefficient A , where the local character is strong, the dynamical exponent may be regarded as $z = \infty$ when we write C_q

in a general form as $C_q = C/q^{z-2}$. By using this expression in $\chi_v^R(q, \omega)$ in the calculation of $\rho(T)$ for $z = \infty$, we obtain $\rho(T) \propto T$ toward $T \rightarrow 0$ K. This result indicates that the locality of valence fluctuations causes the T -linear resistivity. The emergence of $\rho(T) \propto T$ by valence fluctuations was shown theoretically on the basis of the valence susceptibility χ_v which has an approximated form for $z = \infty$ in Ref. [29].

The evaluation of the quasiparticle self-energy for a valence fluctuation exchange process by using the χ_v shows that $\text{Re}\Sigma(\varepsilon) \propto \varepsilon \ln(\varepsilon)$ [30], which leads to a logarithmic- T dependence in the specific heat C/T for a certain- T range [31]. The detailed T dependence of C/T will be discussed in a separate paper.

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