Meta-Orbital Transition in Heavy-Fermion Systems: Analysis by Dynamical Mean Field Theory and Self-Consistent Renormalization Theory of Orbital Fluctuations

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We investigate a two-orbital Anderson lattice model with Ising orbital intersite exchange interactions on the basis of a dynamical mean field theory combined with the static mean field approximation of intersite orbital interactions. Focusing on Ce-based heavy-fermion compounds, we examine the orbital crossover between two orbital states, when the total f-electron number per site $n_f$ is $\sim 1$. We show that a “meta-orbital” transition, at which the occupancy of two orbitals changes steeply, occurs when the hybridization between the ground-state f-electron orbital and conduction electrons is smaller than that between the excited f-electron orbital and conduction electrons at low pressures. Near the meta-orbital critical end point, orbital fluctuations are enhanced and couple with charge fluctuations. A critical theory of meta-orbital fluctuations is also developed by applying the self-consistent renormalization theory of itinerant electron magnetism to orbital fluctuations. The critical end point, first-order transition, and crossover are described within Gaussian approximations of orbital fluctuations. We discuss the relevance of our results to CeAl$_2$, CeCu$_2$Si$_2$, CeCu$_2$Ge$_2$, and related compounds, which all have low-lying crystalline-electric-field excited states.

KEYWORDS: dynamical mean field theory, two-orbital Anderson lattice model, self-consistent renormalization theory, critical end point, orbital fluctuations

1. Introduction

After the discovery of the unconventional superconductivity in CeCu$_2$Si$_2$, various heavy-fermion compounds have attracted great attention. They exhibit many interesting phenomena, such as quantum critical behaviors associated with the quantum critical point (QCP) of magnetic phase transitions under pressure, magnetic field and chemical substitutions, non-Fermi liquid properties near the QCP, and various types of unconventional superconductivity. It is expected that the Cooper pairs in such heavy-fermion superconductors are mediated by magnetic fluctuations, since the superconductivity always occurs near the magnetic phase.

Over the past ten years, the possible nonmagnetic-fluctuation-mediated superconductivity at high pressures separated from the superconductivity near the magnetic QCP has attracted much attention in some heavy-fermion compounds, such as CeCu$_2$Si$_2$, CeCu$_2$Ge$_2$, and related materials, since magnetic fluctuations are not developed there. Near the pressure where the superconducting transition temperature has a peak as a function of pressure, electric resistivity shows a linear temperature dependence, with residual resistivity being enhanced. As pressure increases, Kadowaki-Woods ratio gradually varies from the value for strongly correlated systems to that for weakly correlated systems.

To explain superconductivity without magnetic fluctuations, Onishi and Miyake proposed that Ce-valence fluctuations lead to unconventional superconductivity at high pressures in these systems on the basis of an extended periodic Anderson model (Ex-PAM). The existence of the valence transition in the Ex-PAM was confirmed by more elaborate numerical calculations later. The properties near the critical end point (CEP) of valence fluctuations explain the resistivity and changes in Kadowaki-Woods ratio.

Experimentally, when the f-electron charge per site varies, owing to the electrostatic potential change around a Ce site, the lattice constant should also vary correspondingly, and some of the phonon branches should be affected by this change. However, no direct evidence for the steep changes in Ce valence has been reported.

In this paper, we will focus on the crystalline-electric-field (CEF), i.e., orbital states in these systems. The materials mentioned above all have low-energy excited CEF states. CEF excitations are observed by inelastic neutron scattering experiments. Resistivity data also indicate the existence of excited CEF states, showing a two-peak structure as a function of temperature $T$. The two peaks correspond to two different Kondo temperatures. More importantly, the two peaks merge as pressure increases, and the pressure where the two peaks merge approximately coincides with the pressure where superconducting transition temperature increases as mentioned above. The two-peak structure and its variation as a function of pressure are well explained by the analysis of an orbital-degenerate Anderson lattice model. Interestingly, these behaviors are also observed in CeAl$_2$, which is a prototype of heavy-fermion compounds, at around 3 GPa, while superconductivity has not been observed. A neutron scattering experiment revealed that there are also low-energy CEF states in CeAl$_2$. 
Thus, it is natural to consider that the orbital (CEF) fluctuations in these systems play an important role in realizing the unconventional superconductivity at high pressures. In this paper, we will examine the orbital variations as a function of pressure on the basis of a dynamical mean field theory (DMFT)\(^{19}\) and show that a “metorbital” transition or crossover occurs when hybridizations between conduction and f-electrons depend on the orbital and are sufficiently small compared with the f-electron energy level. We also find that the orbital fluctuations couple with f-electron charge degrees of freedom, leading to the variation in f-electron occupancy when the orbital crossover or transition occurs. We will also try to construct an effective orbital fluctuation theory.

This paper is organized as follows. In §2, a two-orbital Anderson lattice model is analyzed on the basis of a dynamical mean field theory with Wilson’s numerical renormalization group method used as the impurity solver. A theory of critical fluctuations near the critical end point of orbital fluctuations is developed in §3 on the basis of the self-consistent renormalization theory. Finally, §4 shows the summary of the present paper.

2. Two-orbital Anderson Lattice Model with Ising Anisotropic Orbital Interaction

In this section, we investigate orbital fluctuations in a two-orbital Anderson lattice model with Ising orbital intersite exchange interactions on the basis of the DMFT\(^{19}\) combined with the static mean field approximation of intersite exchange interactions. As a solver for the effective impurity problem in the DMFT, we use Wilson’s numerical renormalization group (NRG) method, which is powerful for investigating zero-temperature properties of the impurity problem. We will show the zero-temperature properties of this system, including the variations in the orbital occupancy, the f-electron density of states, and the zero-temperature phase diagram.

2.1 Model

We investigate the periodic Anderson lattice model on a Bethe lattice with two localized f-orbitals (\(\alpha = A \text{ or } B\)) hybridizing with a single conduction electron band.\(^{16}\) We also include Ising orbital-orbital intersite interactions in our model and the Hamiltonian is given as

\[
H = \sum_{ij\sigma}(\epsilon_{ij} - \mu\delta_{ij})c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i\alpha\sigma}v_{i\alpha}(c_{i\sigma}^\dagger f_{i\alpha\sigma} + \text{h.c.}) + (\epsilon_{f\sigma} - \mu)f_{i\alpha\sigma}^\dagger f_{i\alpha\sigma} + \sum_{i\alpha\sigma}U_{\alpha}n_{i\alpha\sigma}n_{i\alpha\sigma} + J_{\alpha}^{2}\sum_{\alpha\sigma}T_{iz}T_{jz}.
\]  

(1)

Here, \(c_{i\sigma}\) and \(f_{i\alpha\sigma}\) represent the annihilation operators for conduction and f-electrons at site \(i\), spin \(\sigma\), and orbital \(\alpha\), respectively. The f-electron number and the orbital occupancy, the f-electron density of states, and the zero-temperature phase diagram.

2.2 Analysis by the dynamical mean field theory

In the DMFT, a lattice model is mapped to an effective impurity one with an effective conduction electron bath.\(^{19}\) In our case, the effective impurity model is an impurity Anderson model with three localized orbitals hybridizing with single-band conduction electrons. In this paper, the intersite orbital interaction is approximated in the mean field level with a uniform amplitude. The effective impurity model is given as

\[
H_{\text{eff}} = \sum_{k\sigma} \left[ \bar{\epsilon_{k}} a_{k\sigma}^\dagger a_{k\sigma} + \left( \frac{\delta_{k\sigma}}{\sqrt{N}} a_{k\sigma}^\dagger c_{\sigma} + \text{h.c.} \right) \right] - \mu \sum_{\sigma} c_{\sigma}^\dagger c_{\sigma} + \sum_{\sigma\sigma'} U_{\sigma} n_{f\alpha\sigma} n_{f\beta\sigma'} - J_{\alpha}^{z}\sum_{\sigma} T_{iz}T_{jz}.
\]  

(2)

Here, \(\bar{\epsilon_{k}}\) includes the contributions of the mean field value of \(\epsilon_{f\alpha}\) and \(\epsilon_{f\beta}\), and \(\epsilon_{f\alpha} = \epsilon_{f\alpha} + J_{\alpha}^{2}\langle T_{iz}\rangle\), where \(\langle \cdots \rangle\) indicates the expectation value and \(\langle T_{iz}\rangle = \langle T_{jz}\rangle\). The operators at the impurity site are defined as \(f_{i\alpha\sigma}^\dagger \equiv f_{i\alpha\sigma}^\dagger f_{i\alpha\sigma}\) and \(c_{\sigma} \equiv c_{\sigma}\). The effective bath is represented by the bath conduction electron \(a_{k\sigma}^\dagger a_{k\sigma}\) hybridizing only with \(c_{\sigma}\). The dispersion and hybridization of the bath conduction electrons are characterized by \(\bar{\epsilon_{k}}\) and
indicating that the dominant orbital occupation changes $\epsilon$ from the $A$-orbital to the $B$-orbital. The variation in $\hat{v}_k$, respectively, which are calculated self-consistently in the DMFT. Although one can integrate both $a_{k\sigma}$ and $c_\sigma$ in a path-integral formulation, it is useful to employ the form (2) for NRG calculations.

To solve the impurity problem in the DMFT, we employ Wilson’s NRG method,20,21 which is powerful for investigating the low-energy properties of the impurity problem. To calculate one-particle Green’s functions correctly, we use the full-density-matrix NRG developed recently.22,23 In the Bethe lattice, the self-consistent equation of the DMFT reads

$$\Delta(\omega) = \frac{1}{N} \sum_k \left| \hat{v}_k \right|^2 \frac{1}{\omega - \epsilon_k} = \frac{1}{4} G_c(\omega),$$  

(3)

where $G_c(\omega) = -i \int_0^\infty dt e^{-i\omega t} \langle T\{c_\sigma(t), c_\sigma^\dagger(0)\} \rangle$ being the local retarded Green’s function for conduction electrons. In the NRG calculations in the DMFT self-consistent loops, we use the logarithmic discretization parameter $\Lambda = 1.8$ and mainly keep 300 low-energy states at each NRG iteration.20 We also confirm that the results do not change when we increase the number of retained states up to 700.

2.2.1 Meta-orbital transition

In this subsection, we will show the numerical results of DMFT+NRG calculations. We will demonstrate that a meta-orbital transition and crossover occur in this system. We will also demonstrate that the orbital degrees of freedom couple with the $f$-electron charge ones.

Figure 1 shows the $\epsilon_{FB}$ dependence of orbital occupancy $\langle T_z \rangle$ for seven sets of $v_B$ with fixed $v_A = 2v_B$. As $\epsilon_{FB}$ decreases, $\langle T_z \rangle$ decreases from $\sim 1$ to $\sim -1$, indicating that the dominant orbital occupation changes from the $A$-orbital to the $B$-orbital. The variation in $\langle T_z \rangle$ as a function of $\epsilon_{FB}$ is gradual when $v_B = 0.5v_A$ is large, while it becomes steeper as $v_B$ decreases. Finite $J_0^z$ also enhances this steep change. Orbital occupancies for $J_0^z = 0.0$ with $v_B = 0.1$ (squares) and $v_B = 0.09$ (filled squares) change smoothly, while those for $J_0^z = 0.02$ with the same parameters show much steeper changes. A CEP is located between $v_B = 0.095$ and 0.1 for $J_0^z = 0.02$. For $v_B = 0.09$, a first-order transition occurs. One can see a clear hysteresis, as shown in Fig. 1. For $v_B = 0.095$, although we have not detected a hysteresis in our calculation, it seems that there is a first-order transition.

These behaviors are analogues of metamagnetism. In the present system, $\epsilon_{FB}$ and $\langle T_z \rangle$ correspond to the magnetic field and magnetization in the language of metamagnetism, respectively. This meta-orbital transition is expected to occur in systems with several low-energy CEF states as the pressure increases. When the parameters are tuned, the CEP is realized. In Fig. 1, we also show the expected variations in $v_B$, $\epsilon_{FB}$, and $\langle T_z \rangle$ in Ce-based compounds, with increasing pressure, indicated by an arrow for $J_0^z = 0.02$. Note that, as the pressure increases, both the hybridization and $f$-electron energy levels are expected to increase in Ce-based heavy-fermion compounds.

Figure 2 shows the $\epsilon_{FB}$ dependences of the total $f$-electron number $n_f$ and the conduction electron number $n_c$ with fixed $n = n_f + n_c = 1.8$. Note that, for $v_B \leq 0.1$, $n_f$ is close to 1 for a small $\epsilon_{FB}$, while $n_f \simeq 0.9-0.95$ for a large $\epsilon_{FB}$. This is because $v_B < v_A$. When $\epsilon_{FB}$ is sufficiently small, for example, $\epsilon_{FB} = -0.55$ and $v_B = 0.095$, $n_f$ decreases from 0.95 to 0.9, while $n_c$ increases from 1.8 to 1.9. The variation in $n_f$ is consistent with the theoretical prediction, as shown in Fig. 2.

Fig. 1. (Color online) $\langle T_z \rangle$ vs $\epsilon_{FB}$ for several values of $v_B = 0.5v_A$, $\epsilon_{FA} = -0.5$, and $J_0^z = 0.0$ and 0.02, and the filling is fixed to be $n = 1.8$. The arrow indicates the typical variation in $\langle T_z \rangle$ for $J_0^z = 0.02$ as a function of pressure for Ce-based heavy-fermion systems.

Fig. 2. (Color online) (a) $n_f$ vs $\epsilon_{FB}$ and (b) $n_c$ vs $\epsilon_{FB}$ for several values of $v_B = 0.5v_A$. The other parameters are the same as those in Fig. 1.
As for the symmetry, the orbital, f-electron number, and conduction electron number belong to the same irreducible representation (scalar). Thus, as shown in Fig. 2, when the meta-orbital transition or crossover occurs, the f-electron number changes accordingly. We note that, across the transition and the crossover, the f-electron number is still close to 1, when \( v_A \) and \( v_B \) are not very large as expected in heavy-fermion systems. This point contrasts the results of the valence transition driven by the Coulomb repulsion between the f- and conduction electrons, \( U_{fc} \), in the Ex-PAM, where a large variation in f-electron number occurs, owing to the large \( U_{fc} \) assumed.\(^{10–12}\)

### 2.2.2 Variation in density of states

Figure 3 shows the density of states (DOS) of f-electrons \(-\text{Im} G_{fA,B}(\omega)/\pi\) for \( v_B = 0.1 = 0.5 v_A \) and several values of \( \varepsilon_{fB} \). Here, \( G_{fA,B}(\omega) \) represents the local A(B)-orbital f-electron retarded Green’s function with the energy \( \omega \). In addition to the lower Hubbard-like peak located at the energy \( \omega \sim \varepsilon_{fA,B} \sim -0.5 \), there are several peaks in the low-energy region, reflecting the CEF excited states. The low-energy peak near \( \omega \sim 0.2 \) in the DOS of the B-orbital for \( \varepsilon_{fB} = -0.44 \) moves to a lower energy as \( \varepsilon_{fB} \) decreases, while a peak appears at a positive energy in the DOS of the A-orbital as \( \varepsilon_{fB} \) decreases, reflecting the meta-orbital crossover discussed previously. There is a sharp peak near \( \omega = 0 \) in \(-\text{Im} G_{fA,B}(\omega)/\pi\). One can also see that there is a hybridization gap like structure for the A(B)-orbital DOS when \( \varepsilon_{fB} \) is larger (smaller) than approximately \( \varepsilon_{fB} \sim -0.53 \), as shown in Figs. 3(b) and 3(c).

To investigate the low-energy DOS in more detail, we show the DOS at \( \omega = 0 \) as a function of \( \varepsilon_{fB} \) in Fig. 4, where we define \( G_{\text{tot}} = G_{fA} + G_{fB} + G_c \). Since \( \text{Im} G_c \) does not show notable changes, we do not show it. The DOS of the A-orbital at \( \omega = 0 \) is large when \( \varepsilon_{fB} \) is large, while it is small when \( \varepsilon_{fB} \) is small. Correspondingly, the DOS of the B-orbital at \( \omega = 0 \) is large for a small \( \varepsilon_{fB} \) and small for a large \( \varepsilon_{fB} \). In Fig. 4, one can also see a clear hysteresis in the DOS at \( \omega = 0 \) for \( v_B = 0.09 \).

If we employ the variations in hybridization and f-electron level as pressure increases as shown by the arrow in Fig. 1, we observe that the DOS at the Fermi level decreases as pressure increases. The steepness of this variation depends on the distance to the CEP from the parameter path that corresponds to the physical pressure.

![Fig. 3.](image-url) (Color online) (a) f-electron density of states vs \( \omega \) for \( v_B = 0.1 \) and \( v_A = 0.2 \) for several values of \( \varepsilon_{fB} \). Full and dashed lines represent the DOS for the A- and B-orbitals, respectively. The values of \( \varepsilon_{fB} \) decrease from bottom to top as \( \varepsilon_{fB} = -0.44, -0.45, -0.46, -0.47, -0.48, -0.49, -0.50, -0.505, -0.51, -0.515, -0.52, -0.525, -0.528, -0.53, -0.532, -0.535, -0.538, -0.542, -0.547, -0.555, \) and \(-0.56 \). Each line is shifted by 0.3. The other parameters are the same as those in Fig. 1. (b) Low-energy structure of A-orbital density of states. (c) Low-energy structure of B-orbital density of states.

### 2.2.3 Phase diagram

To summarize this section, we show the schematic ground state phase diagram of the two-orbital Anderson model with two different hybridizations (\( v_B < v_A \)) and ferro-orbital intersite interactions in Fig. 5. As discussed above, we observe a first-order transition line and its CEP. In Fig. 5, the “A(B)-rich” region indicates the region with a larger f-electron occupancy in the A(B)-orbital. The “A-rich” region is located in the larger \( \varepsilon_{fB} \) region, where the effective mass is smaller than that in the “B-rich” region, owing to the large \( v_A > v_B \). We also call it “light” Fermi liquid instead of heavy Fermi liquid. This light Fermi liquid can be regarded as the state with larger valence fluctuations than the B-rich state, since \( v_A > v_B \). Near the CEP, f-electron charge fluctuations and also conduction electron ones are enhanced. The effective mass also changes steeply near the CEP, reflecting the variation in orbital occupancy.

Since our analysis is based on the DMFT and the mean field approximation for intersite orbital interactions \( J_{z}^z \), we overestimate the effects of \( J_{z}^z \). As shown in Fig. 1, the \( \varepsilon_{fB} \) dependence of \( (T_z) \) for \( J_{z}^z = 0 \) is much weaker than that for \( J_{z}^z = 0.02 \). We have not carried out DMFT+NRG calculations for a very small \( v_B < 0.09 \), since very small hybridizations make the NRG calculation difficult. When \( J_{z}^z \rightarrow 0 \), whether the first-order transition occurs or not is beyond the scope of the present
analysis. However, it is noted that when one of the hybridizations is zero, there must be a first-order transition even when $J_0 = 0$. To clarify whether this first-order transition exists in the region where the hybridization is finite, more elaborate numerical calculations that can take into account the intersite correlations are needed.

As for magnetic instabilities, it is expected that magnetic phases will appear in the phase diagram, especially in the region of the smaller $v_B$ and $\varepsilon_{FB}$, corresponding to the low-pressure region in typical Ce-based heavy-fermion systems. Determining the phase diagram including the magnetic phases and their magnetic structures is beyond the scope of the present paper and we leave it as a future study. It is also interesting to investigate the case that the magnetic transition and the orbital CEP occur simultaneously. Such a situation might lead to a new universality class of magnetic phase transitions.

3. Self-Consistent Renormalization Theory of Nonmagnetic Orbital Fluctuations

In this section, we will develop a self-consistent renormalization theory for the orbital fluctuations discussed in §2 on the basis of the DMFT. Since the DMFT does not take into account the long wavelength fluctuations, we use the one-loop self-consistent approximation scheme of the fluctuations known as the self-consistent renormalization (SCR) theory developed by Moriya and Kawabata for itinerant electron magnetism.24–26 When we apply the SCR theory to the nonmagnetic orbital fluctuations, we need to take into account the temperature dependence of the order parameter itself and the temperature dependence originating from the order parameter in the mode-coupling corrections. Our discussion in this section leads to results similar to those of the SCR theory for meta-magnetic fluctuations27 and Kondo-volume-collapse transition in heavy-fermion systems.28 It is noted that our formulation naturally describes both the order parameter and the mode-coupling corrections in an equal footing based on a variational principle. We will discuss the orbital fluctuations in three-dimensional ($d = 3$) systems in this paper, although the application to the cases with $d \neq 3$ is straightforward.

3.1 Landau-Ginzburg-Wilson action

The Landau-Ginzburg-Wilson action for nonmagnetic fluctuations generally has odd order terms with respect to field variables, which is given as

$$S = \sqrt{\frac{N}{T}} h \phi_0 + \frac{1}{2} \sum_p a_p \phi_p \phi_{-p}$$

$$+ b \sqrt{\frac{T}{N}} \sum_{p_1p_2} \phi_{p_1} \phi_{p_2} \phi_{-p_1-p_2}$$
Here, \( \phi_p \) is the nonmagnetic field with \( \phi_p^* = \phi_{-p} \) and \( p \) represents the momentum and energy. \( N \) and \( T \) are the number of lattice sites and temperature, respectively. In terms of \( S \), the free energy \( F \) is given by \( \exp(-F/T) = \int \mathcal{D}\phi \exp(-S) \). We neglect the momentum and energy dependence of the coefficients \( b \) and \( c \), which are irrelevant from simple power counting in the context of the renormalization group. For the stability of the system, \( c > 0 \), \( \dot{\phi} \) is the field conjugate to the uniform nonmagnetic field \( \phi_0 \); thus, does not depend on \( p \). Since we are interested in the orbital transition without breaking translational symmetry, we use the Ornstein-Zernike form of \( a_p \) as in the ferromagnetic fluctuation: 24-26

\[
a_p = a_0 + A|q|^2 + C|\omega_n|/|q|,
\]

where \( q \) and \( \omega_n \) are the momentum and the Bosonic Matsubara frequency, respectively. Existence of the odd order terms in eq. (4) leads to the first-order transition, CEP, and also crossover, as shown in Fig. 5.

3.2 Modified SCR theory

In the SCR theory, the non-Gaussian terms in the free energy \( F \) are approximated by mean field decoupling. 24-26, 29 This approximation corresponds to variationally determining the coefficients of the Gaussian fluctuations. In our case with the presence of \( h \) and \( b \) terms, we need to take into account the order parameter itself in addition to mode-coupling terms. We will show that a modified Gaussian action can describe the first-order transition, the CEP, and the crossover.

To describe the order parameter variations within the Gaussian approximation, we assume the following variation action:

\[
S_{\text{eff}} = \frac{1}{2} \sum_{p \neq 0} r_p \dot{\phi}_p \dot{\phi}_{-p} + \sqrt{\frac{N}{T}} \hat{h} \phi_0 + \frac{1}{2} \dot{\phi}_0^2,
\]

\[
r_p = a_p + \delta,
\]

where \( \delta \) and \( \hat{h} \) are variational parameters. On the basis of Gibbs-Bogoliubov-Feynman inequality, they are determined by minimizing \( \tilde{\Omega} \):

\[
\tilde{\Omega} = \Omega_{\text{eff}} + T\langle S - S_{\text{eff}} \rangle,
\]

\[
\Omega_{\text{eff}} = -T \log Z_{\text{eff}},
\]

\[
Z_{\text{eff}} = \int \mathcal{D}\phi \exp(-S_{\text{eff}}),
\]

\[
\langle S \rangle = \int \mathcal{D}\phi S \exp(-S_{\text{eff}})/Z_{\text{eff}}.
\]

Defining the order parameter \( \phi \) as \( \phi = \sqrt{T/N} \phi_0 \), we obtain

\[
\frac{\tilde{\Omega}}{N} = \frac{\Omega_{\text{eff}}}{N} + (h - \hat{h})\langle \phi \rangle - \frac{\delta}{2} \langle \phi^2 \rangle + b\langle \phi^3 \rangle + c\langle \phi^4 \rangle + 3(b\langle \phi \rangle + 2c\langle \phi^2 \rangle)\frac{T}{N} \sum_{p \neq 0} \frac{1}{r_p} - \frac{\delta}{2} T \frac{N}{2} \sum_{p \neq 0} \frac{1}{r_p}
\]

\[
+ 3c\left( \frac{T}{N} \sum_{p \neq 0} \frac{1}{r_p} \right)^2.
\]

Since the effective action \( S_{\text{eff}} \) is Gaussian, we can analytically calculate \( \langle \phi^n \rangle \) with \( n \) being any integers, and they are given as

\[
\langle \phi \rangle = -\frac{\hat{h}}{r_0},
\]

\[
\langle \phi^2 \rangle = \frac{T}{N} \frac{1}{r_0} + \frac{\hat{h}^2}{r_0} = \frac{T}{N} \frac{1}{r_0} + \langle \phi \rangle^2,
\]

\[
\langle \phi^3 \rangle = -\frac{T}{N} \frac{3\hat{h}}{r_0} - \frac{\hat{h}^3}{r_0} = 3\langle \phi^2 \rangle \langle \phi \rangle - 2\langle \phi \rangle^3,
\]

\[
\langle \phi^4 \rangle = -\frac{T^2}{N^2} \frac{3\hat{h}}{r_0} - \frac{T}{N} \frac{6\hat{h}^2}{r_0} + \frac{\hat{h}^4}{r_0} = 3\langle \phi^2 \rangle^2 - 2\langle \phi \rangle^4.
\]

Differentiating \( \tilde{\Omega}_{\text{eff}} \) with respect to \( \delta \), we obtain

\[
\left[ h - \hat{h} + 3b\frac{T}{N} \sum_{p \neq 0} \frac{1}{r_p} + 3b\langle \phi^2 \rangle - 8c\langle \phi^3 \rangle - 6b\langle \phi \rangle^2 \right] \frac{\partial \langle \phi \rangle}{\partial \delta}
\]

\[
+ \left[ -\frac{\delta}{2} + 6c \frac{T}{N} \sum_{p \neq 0} \frac{1}{r_p} + 3b\langle \phi \rangle + 6c\langle \phi^2 \rangle \right] \times \frac{\partial}{\partial \delta} \left[ \langle \phi^2 \rangle + \frac{\sum_{p \neq 0} \frac{1}{r_p}}{N} \right] = 0.
\]

Using eq. (15) and defining

\[
X = \frac{T}{N} \sum_{p \neq 0} \frac{1}{r_p},
\]

we obtain

\[
\left[ h - \hat{h} + 3bX - 3b\langle \phi \rangle^2 - 8c\langle \phi \rangle^3 \right] \frac{\partial \langle \phi \rangle}{\partial h}
\]

\[
+ \left[ -\frac{\delta}{2} + 6cX + 3b\langle \phi \rangle + 6c\langle \phi \rangle^2 \right] \frac{\partial}{\partial h} \langle \phi \rangle^2 = 0.
\]

Note that when \( h = \hat{h} = b = \langle \phi \rangle = 0 \), eq. (20) leads to the self-consistent equation

\[
\delta = 12cX,
\]

which coincides with the conventional expression. 24, 26 Similarly, differentiating \( \Omega_{\text{eff}} \) with respect to \( \hat{h} \) leads to

\[
\left[ h - \hat{h} + 3bX - 3b\langle \phi \rangle^2 - 8c\langle \phi \rangle^3 \right] \frac{\partial \langle \phi \rangle}{\partial \hat{h}}
\]

\[
+ \left[ -\frac{\delta}{2} + 6cX + 3b\langle \phi \rangle + 6c\langle \phi \rangle^2 \right] \frac{\partial}{\partial \hat{h}} \langle \phi \rangle^2 = 0.
\]
Combining eqs. (20) and (22), we obtain
\[
\hat{h} = h + 3bX - 3b\langle \phi \rangle^2 - 8c\langle \phi \rangle^3, \tag{23}
\]
\[
\delta = 12cX + 6b\langle \phi \rangle + 12c\langle \phi \rangle^2. \tag{24}
\]
Equations (23) and (24) are the self-consistent equations in our theory.

Now, we derive the equation of state for \(\langle \phi \rangle\). Using eqs. (14), (23), and (24), the equation of state is derived as
\[
h + 3bX + (a_0 + 12cX)\langle \phi \rangle + 3b\langle \phi \rangle^2 + 4c\langle \phi \rangle^3 = 0. \tag{25}
\]
Parameterizing \(\langle \phi \rangle = \delta \phi - b/(4c)\) for later purposes, eq. (25) is rewritten as
\[
\left[ h - \frac{a_0b}{4c} + \frac{2b^3}{(4c)^2} \right] + \left( a_0 - \frac{3b^2}{4c} + 12cX \right) \delta \phi + 4c\delta \phi^3 = 0. \tag{26}
\]
Equation (26) is the basic equation used to determine the order parameter \(\delta \phi\). Note that \(\delta \phi\) appears only in the form of \(\delta \phi^2\) in \(X\) from the definition of \(\delta \phi\) and eq. (24), and the effect of fluctuations on \(h\) in eq. (25) is canceled out by the shift of \(\phi \rightarrow \delta \phi - b/(4c)\). The fluctuation term appears only in the coefficient of \(\delta \phi\) in eq. (26). This equation describes the first-order transition, the CEP, and also the crossover while taking into account the mode-coupling correction \(X\) within the Gaussian fluctuation theory. A similar equation of state was introduced in ref. 28, where the renormalization of \(h\) was neglected in eq. (25).

Figure 6 shows the temperature and \(h\) dependences of the order parameter \(\delta \phi\). Here, the critical value \(a_{0c}\) is given by eq. (36) and the parameters \(T_0, T_A, x_c\) introduced in Appendix B are fixed as \(T_0 = 20\) K, \(T_A = 50\) K and \(x_c = 300\). In Fig. 6(a), there is a first-order transition for \(h/2T_A \sim 0.05749\) below \(T/T_0 = 0.01\). In Fig. 6(b), the parameter \(a_0\) is fixed as \(a_0 = a_{0c}\); and thus, at zero temperature, the CEP is realized at \(h \sim 0.05476\). In Figs. 6(c) and 6(d), there is no phase transition and \(\delta \phi\) varies smoothly as functions of \(T\) and \(h\).

### 3.3 Zero-temperature critical end point

In this subsection, we investigate the nonmagnetic orbital fluctuations near the zero-temperature CEP in detail. Details of the calculations are summarized in Appendix B.

Near the zero-temperature CEP, \(r_0 \sim 0\), \(X\) in eq. (19) is expanded in terms of \(r_0\) as
\[
X = K_0 + K_1 r_0 + K(T), \tag{27}
\]
with
\[
r_0 = a_0 + 12c[K_0 + K_1 r_0 + K(T)] - \frac{3b^2}{4c} + 12c\delta \phi^2,
\]
\[
= \frac{1}{1 - 12cK_1} \left[ a_0 - \frac{3b^2}{4c} + 12c\delta \phi^2 + 12c(K_0 + K(T)) \right],
\]
and
\[
K_0 > 0, \quad K_1 < 0, \quad \text{and} \quad K(T) > 0. \tag{29}
\]
As is well known, \(K(T) \propto T_{4/3}\) in three-dimensional systems with the dynamical exponent \(z = 3^{24,26}\) (see Appendix B). Now, substituting eqs. (27) and (28) into eq. (26), we obtain
\[
H_0 + \left[ A_0 + A_1 K(T) \right] \delta \phi + 4c_0 \delta \phi^3 = 0, \tag{30}
\]
where
\[
H_0 = \hat{h} - \frac{a_0b}{4c} + \frac{2b^3}{(4c)^2}, \tag{31}
\]
\[
A_0 = a_0 - \frac{3b^2}{4c} + \frac{12cK_1}{1 - 12cK_1} \left[ a_0 - \frac{3b^2}{4c} + \frac{K_0}{K_1} \right], \tag{32}
\]
\[
A_1 = \frac{12c}{1 - 12cK_1} > 0, \tag{33}
\]
\[
4c_0 = 4c \left[ 1 + \frac{36cK_1}{1 - 12cK_1} \right]. \tag{34}
\]
In the case that the \(\delta \phi\) dependence of \(K_0, K_1, \text{and} K(T)\) is negligible, eq. (30) can be derived by minimizing the effective free energy \(F_{\text{eff}}\) given as
\[
F_{\text{eff}} = H_0 \delta \phi + \frac{1}{2} \left[ A_0 + A_1 K(T) \right] \delta \phi^2 + C_0 \delta \phi^4, \tag{35}
\]
which is nothing but the Landau’s free energy for ferromagnetism in the presence of the magnetic field \(-H_0\).

Since \(K(T)\) vanishes at the zero-temperature CEP as \(T_{4/3}\), the zero-temperature CEP is realized when \(H_0 = A_0 = 0\), which is equivalent to \(r_0 = 0\) and \(h = 0\). As a result, the critical value of the order parameter is \(\delta \phi = 0\), leading to \(\langle \phi \rangle = -b/(4c)\). In terms of the original parameters, we obtain the conditions for the zero-
temperature CEP as
\[ a_{0c} = \frac{3b^2}{4c} - 12cK_0, \quad (36) \]
\[ h_c = \frac{b^3}{(4c)^2} - 3bK_0, \quad (37) \]
at zero temperature. Using eqs. (36) and (37), eqs. (31) and (32) are rewritten as
\[ H_0 = h - h_c, \quad (38) \]
\[ A_0 = \frac{(a_0 - a_{0c}) (1 + 12cK_1)}{1 - 12cK_1}, \quad (39) \]

Let us discuss the temperature dependence of \( \delta \phi \) near the zero-temperature CEP in the case of \( C_0 > 0 \) as expected for a small \( c > 0 \).

First, we consider the case that all the parameters, \( h, a_0, b, c, A, \) and \( C \) are constant, i.e., temperature-independent. Then, \( H_0 = 0 \) and \( A_0 = 0 \) in eq. (30), when the CEP is realized at zero temperature. We obtain \( \delta \phi = 0 \) or
\[ \delta \phi^2 = \frac{-A_1(0)}{4C_0(0)}K(T), \quad (40) \]
where \( A_1(0) \) and \( C_0(0) \) are the zero-temperature values of \( A_1 \) and \( C_0 \), respectively. Since \( A_1(0) > 0 \), \( K(T) > 0 \), and \( C_0(0) > 0 \), the solutions of eq. (40) are pure imaginaries. Thus, \( \delta \phi = 0 \) for all temperatures without taking into account the temperature dependence in the parameters. This corresponds to the order parameter variation in Fig. 6(b) for \( h/2TA \sim 0.05746 \).

Secondly, we consider that the leading temperature dependence of the parameters is proportional to \( T^2 \) as expected in Fermi liquid states. In this case, eq. (30) becomes
\[ A_1(0)K(T)\delta \phi + 4C_0(0)\delta \phi^3 \approx -H_0''T^2, \quad (41) \]
where \( H_0 \approx H_0''T^2 \). Thus, we obtain \( \delta \phi \propto T^{2/3} \), since this temperature dependence is self-consistent with \( K(T) \propto T^{4/3} \). Setting \( K(T) = \kappa T^{4/3} \) with \( \kappa > 0 \), and \( \delta \phi = \varphi T^{2/3} \), we obtain
\[ A_1(0)\kappa \varphi + 4C_0(0)\varphi^3 \approx -H_0''. \quad (42) \]
When \( A_1(0) > 0 \) and \( C_0(0) > 0 \), eq. (42) always has only one solution \( \varphi \), which is either positive or negative, depending on the sign of \( H_0'' \). The first-order transition occurs as \( H'' \) changes for \( A_1(0) < 0 \) and \( C_0(0) > 0 \).

It is noted that \( \phi \) couples any quantities and thus, in general, this nonanalytic temperature dependence \( \delta \phi \propto T^{2/3} \) appears in any physical observables near the zero-temperature CEP. For example, the magnetic susceptibility \( \chi_s \) has, rather than the usual \( T^2 \) dependence, the nonanalytic temperature dependence as
\[ \chi_s^{-1}(T) \approx \chi_s^{-1}(0) + \lambda \delta \phi + \cdots. \quad (43) \]

Here, \( \lambda \) is the coupling constant between magnetic and nonmagnetic fluctuations such as \( \lambda \delta \phi \sum_p M_p M_{-p} \) in the action, where \( M_p \) is the magnetic fluctuation at the momentum and the energy \( p \). Thus, there might be a finite temperature region where \( \chi_s(T) \propto T^{-2/3} \) is observed, when \( \chi_s^{-1}(0) \) is suppressed by some factors. Since the present theory is phenomenological, the microscopic discussions on this issue are beyond the scope of this paper.

As for the other thermodynamic and transport quantities, we obtain the same critical behaviors as those in the ferromagnetic QCP with \( z = 3 \) and \( d = 3 \). The specific heat coefficient diverges as \( C/T \sim -\log T, \quad (31) \) and the resistivity is given as \( \rho \sim T^{5/3}, \quad (32) \) in the asymptotic limit. It is noted that, at a higher temperature, \( \rho \propto T \) as is the case for all the bosonic fluctuations.

### 3.4 Critical end point at finite temperature

Here, we discuss the temperature dependence of \( \delta \phi \) near a finite-temperature CEP at \( T = T^* > 0 \).

As in the case of the zero-temperature CEP discussed in §3.3, we first consider the case that all the parameters have no temperature dependence. In this case, \( \delta \phi = 0 \) for \( T > T^* \) and \( \delta \phi \propto \sqrt{K(T^*) - K(T)} \) for \( T < T^* \). Thus, we obtain \( \delta \phi \propto (T^* - T)^{1/2} \) near \( T \sim T^* \), exhibiting the mean field behaviors. This is understood by noting that our theory is essentially mean field approximation and that the \( H_0 = 0 \) line in the parameter space corresponds to the case of the Ising model without magnetic fields, identifying \( A_0 + A_1K(T) \) as \( T - T_c \), where \( T_c \) is the magnetic transition temperature.

In the second case, the temperature dependence of all the parameters is proportional to \( T^2 \) as derived in Fermi liquid states. Expanding the temperature dependence from the critical end point temperature \( T^* \), we obtain
\[ 0 \approx \left. \frac{\partial H_0}{\partial T} \right|_{T=T^*} (T - T^*) + 4C_0(T^*)\delta \phi^3. \quad (44) \]

Here, we assume \( T^* \ll T_{FL} \), where \( T_{FL} \) is the so-called Fermi liquid temperature below which the Fermi liquid behaviors appear. In eq. (44), the temperature dependence in the second term in eq. (26) or (30) is on the higher order in \( (T^* - T^*)/T^* \), and thus we neglect it. Then, the asymptotic temperature dependence of the order parameter \( \delta \phi \) near the finite-temperature CEP is
\[ \delta \phi = \pm \left. \frac{1}{4C_0(T^*)} \frac{\partial H_0}{\partial T} \right|_{T=T^*} \frac{T^* - T}{T^* - T}. \quad (45) \]

Comparing this with the result at the zero-temperature CEP as discussed in Sec. 3.3, one can see that there is a classical-quantum crossover from \( \delta \phi \propto |T - T^*|^{1/3} \) to \( \delta \phi \propto T^{2/3} \) as \( T^* \) decreases in the second case.

Physically, it is unrealistic to consider \( H_0 = 0 \) for all temperatures in real materials; thus, the second case is more realistic for experimental situations. However, the first case is pedagogically important, since it clearly exhibits this transition belonging to the Ising-type universality class as expected. It is also important to note that \( \delta \phi \propto T^{2/3} \) is realized only when \( T_{FL} \) is well defined, i.e.,
when the Fermi liquid theory is valid and the condition $T/T_{FL} \ll 1$ is realized.

4. Discussion and Summary

We have discussed orbital fluctuations in a two-orbital Anderson lattice model on the basis of the DMFT in §2 and constructed a self-consistent critical theory of the orbital fluctuations in §3.

In the first part of this paper in §2, we have investigated meta-orbital transition in the two-orbital Anderson model with anisotropic intersite orbital-orbital interactions, and the schematic phase diagram is shown in Fig. 5 as the summary of §2.

First, our results demonstrate that a meta-orbital transition or crossover with steep changes in orbital occupancy occurs as pressure increases, only when the hybridization between the conduction electrons and the f-electrons at ambient pressure is sufficiently small. For simplicity, let us consider that the pressure affects the electrons at ambient pressure is sufficiently small. For example, phonon scatterings lead to such a temperature dependence should be cut off at the scale $T_A$, below which the asymptotic behaviors characteristic to $d = 3$ and $z = 3$ discussed above appear.

As for the temperature dependence of the resistivity, it is shown$^7$ that the valence fluctuations lead to the $T$-linear dependence near the CEP, assuming a small $A$ in eq. (5) from the results of the slave boson theory.$^{10}$ It is noted that the $T$-linear temperature dependence is realized in all the bosonic fluctuations at high temperatures. For example, phonon scatterings lead to such a behavior at high temperatures. In the case of the orbital fluctuations, it is not clear whether the $A$ coefficient needs a more quantitative analysis. When $A \sim 0$ in eq. (5), we obtain $K(T) \propto T^{2/3}$ near the CEP$^{33}$ and the equation of state (30) leads to $\delta \phi \propto T^{3/3}$ when all the parameters vary as a function of $T^2$ at low temperatures. Note that this temperature dependence should be cut off at the scale $T_A$, below which the asymptotic behaviors characteristic to $d = 3$ and $z = 3$ discussed above appear.

In our theory, it is expected that CeCu$_2$Si$_2$ and related compounds and CeAl$_2$ at ambient pressure are on the left side of the line of the first-order transition in Fig. 5, i.e., in the $B$-rich phase. As for superconductivity, it is expected that compounds that show superconductivity away from their magnetic QCP pass near the CEP in Fig. 5 as pressure increases, while nonsuperconducting materials, such as CeAl$_2$, are not sufficiently close to the CEP, assuming that magnetic phases exist on the left side in the phase diagram in Fig. 5. Since there are many aspects that affect the realization of superconductivity, such as the energy scale of the fluctuations and band structures,$^{34}$ more quantitative model and analysis are needed in order to clarify the details of the superconductivity realized in these systems.
In summary, we have investigated orbital fluctuations in heavy-fermion systems. We have shown that a meta-orbital transition occurs as pressure increases and the orbital variations affect the density of states at the Fermi level and also f-electron occupancy. We have also constructed an effective critical theory for the orbital fluctuations, which describes both the first-order transition and crossover on the basis of a variational principle. Our results give a possible scenario for the superconductivity and non-Fermi liquid behaviors associated with orbital fluctuations in heavy-fermion systems.

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Appendix A: Localized limit and intersite interactions

In this appendix, we will derive the intersite orbital interaction via a fourth-order perturbation in $v_{\alpha}$ from the localized limit of the Hamiltonian (1) without the $J^z_\alpha$ term. Note that $J^z_\alpha$ is not exactly the same as the orbital intersite interaction that will be derived in this appendix. $J^z_\alpha$ has been introduced phenomenologically in order to take into account the intersite orbital correlation in the DMFT calculation in §2.

Let us consider Hamiltonian (1) without $J^z_\alpha$. In the limit of $U_{\alpha}$, $U' \to \infty$, and $v_{\alpha} \to -\infty$ keeping $U_{\alpha}/|\varepsilon_{f\beta}| \gg 1$ and $v_{\alpha}v_{\beta}/|\varepsilon_{f\gamma}|$ finite, the local excited configuration of $\Phi$ contributes to the low-energy properties of this system only as virtual states and configurations with $\Phi'(n \geq 2)$ are neglected. Thus, the effective Hamiltonian can be written by the localized spin and orbital degrees of freedom interacting with conduction electrons via exchange interactions:

$$H_{ex} = \sum_{i,j} (-t_{ij} - \mu \delta_{ij}) c^\dagger_{i\sigma} c_{j\sigma} + \sum_{i\sigma} J_{\alpha} c^\dagger_{i\sigma} (s^E)_{\sigma\sigma'} c_{i\sigma'} \cdot S_i + \Delta \sum_i T_{iz} + \sum_{i,\sigma,\sigma'} J_{AB} c^\dagger_{i\sigma} (s^E)_{\sigma\sigma'} c_{i\sigma'} T_{iz} \cdot S_i + K_{AB} \sum_i n_{ic} T_{iz} + K^z_{AB} \sum_i n_{ic} T_{iz},$$

where $S_i$ represents the f-electron spin operator at site $i$ and the conduction electron spin is given as $s^E_{ij} = \sigma_\mu/2$, where $\sigma_\mu$ with $\mu = x, y$ or $z$ is the Pauli matrix. $n_{ic}$ is the conduction electron charge operator $n_{ic} = \sum_{i\sigma} c^\dagger_{i\sigma} c_{i\sigma}$. As for the orbital degrees of freedom of f-electrons, $T_{ix} = \sigma_x$ and $T_{iz} = \sigma_z$ acting on the orbital space at site $i$ and the two eigenvalues of $T_{iz}$ are 1 for the $A$-orbital and $-1$ for the $B$-orbital. The coupling constants are given as

$$J_{\alpha} = \frac{v_{\alpha}^2}{-\varepsilon_f},$$

$$K_{AB}^z = \frac{2 v_A v_B}{-\varepsilon_f},$$

where $\varepsilon_f$ is the conduction electron charge susceptibility.

Here, we assume $\varepsilon_{fA} \sim \varepsilon_{fB} \equiv \varepsilon_f$ and ignore the difference between $\varepsilon_{fA}$ and $\varepsilon_{fB}$ in the denominator of $J_{\alpha}$, $J_{AB}$, $K_{AB}^z$, and $K_{AB}$. The difference is taken into account in $\Delta = \varepsilon_{fA} - \varepsilon_{fB}$.

Now, intersite interactions in the second-order perturbations of $J_{\alpha}, J_{AB}, K_{AB}^z,$ and $K_{AB}$ are obtained straightforwardly. Among them, the Ising-type orbital-orbital interaction is given as

$$K_{AB}^z \sum_{i,j} T_{iz} \chi_{ij} T_{jz},$$

where $\chi_{ij}$ is the conduction electron charge susceptibility. Note that, when $v_B \gg v_A$ (or $v_B \gg v_B$), the coupling constant $J_B$ (or $J_A$) and $|K_{AB}^z|$ is much larger than $J_{AB}$ and $K_{AB}^z$. In this limit, the spin-spin and Ising orbital interactions on the fourth order in $v_{\alpha}$ are more important than those in the other sectors, such as the transverse orbital and spin-orbital coupled interactions.

Appendix B: Detailed calculations in SCR theory

In this appendix, we summarize the detailed calculations of the mode coupling correction $X$ in the SCR theory in order to make this paper self-contained.

Let us parameterize $X$ in eq. (19) as

$$X = \frac{T}{N} \sum_{q,n} \frac{1}{\omega_n + A|q|^2 + C(|\omega_n|q)^{-\phi}},$$

with $\theta = 1$. Following the discussions by Misawa et al.,

$$X = K(0) + K(T),$$

where $K(0) = \frac{K_d}{\pi} \int_{0}^{\infty} dq \int_{0}^{\infty} d\omega \frac{C\omega \epsilon^{t+\epsilon-1}}{[q^2(\phi_0 + A\phi_0^2)]^2 + (C\omega)^2}$

and $K(T) = \frac{2K_d}{\pi} \int_{0}^{\infty} dq \int_{0}^{\infty} d\omega \frac{\epsilon_n B(\omega) \epsilon_n^{t+\epsilon-1}}{[q^2(\phi_0 + A\phi_0^2)]^2 + (C\omega)^2}$

where $\epsilon_n B$ is the Bose distribution function $\epsilon_n B(\omega) = \Gamma [\epsilon_n B(\omega)] = \frac{1}{(\epsilon_n B(\omega) + 1)}$ and $K_d = 2\pi \epsilon^{t/2}/[(2\pi)^d \Gamma(d/2)]$, with $\Gamma$ being the gamma function. In terms of dimensionless parameters, eqs. (B-3) and (B-4) are rewritten as

$$K(0) = \frac{T_{0d}}{T_A} \int_{0}^{\infty} dz' \int_{0}^{\infty} \frac{dx}{x^2} \frac{x^{d+\phi-1}}{x^{2} + z'^2},$$

$$K(T) = \frac{2T_{0d}}{T_A} \int_{0}^{\infty} \frac{dz}{c^{2\pi d}} \int_{0}^{\infty} \frac{dx}{x^2} \frac{x^{d+\phi-1}}{x^2 + z^2}.$$
where $\psi$ is the di-gamma function and $u = x^0(y + x^2)/t$. Rescaling by $t^{1/(2+\theta)}$, eq. (B-7) becomes

$$\mathcal{K}(T) = \frac{T_0 d}{t_A} \int_0^{x_c} dz \left[ \log \left( 1 - \frac{1}{2u} - \psi(u) \right) \right].$$

Here, $u = \alpha(y, t, \theta)s^\theta + s^{2+\theta}$ with $\alpha(y, t, \theta) = y/t^{x/2}$. As discussed by Misawa et al., [29] eq. (B-8) is proportional to $t^{\frac{x}{2+\theta}}$ if $\alpha(y, t, \theta) \to 0$ for $t \to 0$. This is understood by noting that $u \to s^{2+\theta}$ for $t \to 0$ and the integral has no $t$ dependence for a small $t$.

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