Heavy Fermion Physics

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This article is intended to be a very brief review on the most basic facts and concepts of heavy fermion physics. A general overview is given as an introduction. In the following part, the mechanism leading to the formation of heavy fermions is explained briefly, and its connection to Kondo effect is emphasized. Then we talk about heavy fermion theories in more detail, where the concepts like Kondo lattice, slave boson are introduced. Then there are two separate parts on Kondo insulators and heavy fermion superconductivity respectively.

Keywords: heavy fermion, Kondo effect, Kondo insulator, superconductivity

I. INTRODUCTION

Heavy fermion martials are those metallic compounds which have enormously large effective electron masses below certain temperatures. It is well known that, at temperatures much below the Debye temperature and Fermi temperature, the heat capacity of metals can be written as the sum of electron and phonon contributions:

$$C = \gamma T + AT^3 \quad (1)$$

and the electron term is linear in T and dominant at low temperatures. The material-dependent constant γ is proportional to the effective electron mass m^*. In common metals the ratio of this effective mass to the real electron mass is within the order of 10. However, in the late seventies, people discovered some metallic compounds whose m^*s are two or three orders of magnitude higher than usual, which is the origin of the name heavy fermion (Fig 1).

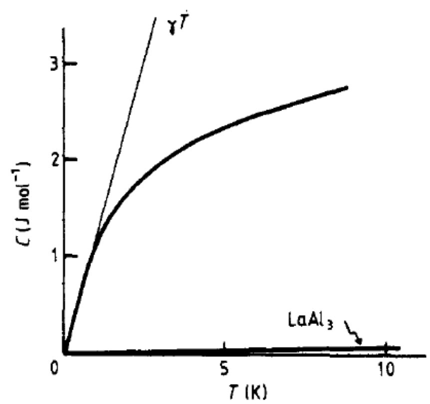

FIG. 1: Schematic plot of the specific heat $C(T)$ for $CeAl_3$. For comparison we show also the results for the related compound $LaAl_3$. The specific heat coefficient γ of $CeAl_3$ is of order $J{\cdot}mol^{-1}K^{-2}$, instead of order $mJ{\cdot}mol^{-1}K^{-2}$ as in ordinary metals. [1]

The first material of this kind in history is $CeAl_3$ alloy, which was discovered by Andres, Graebner and Ott [2] in 1975. Since then, bunch of other heavy fermion materials have been discovered and studied, which include $CeCu_2Si_2$, $CeCu_6$, UBe_{13}, UPt_3, UCd_{11}, U_2Zn_{17}, $NpBe_{13}$, etc. Among them, there are superconductors, antiferromagnets and insulators. However, one common property of these compounds is that one of the constituents of each is a rare-earth or actinide atom with partially filled $4f$- or $5f$-electron shells. At high temperatures the f-electrons are localized on their atomic sites and do not contribute to conduction. However, contrary to conventional materials, some of the f-electrons become itinerant at low temperatures. Crudely speaking, it is these itinerant f-electrons that lead to the uncommon behaviors of heavy fermion materials at low temperatures. We will go to detail in Sec. II.

One distinctive property of heavy fermion materials is that in these systems quantum fluctuations of the magnetic and electronic degrees are strongly coupled to each other, which may lead to quite a lot of unconventional behaviors. Moreover, as one of the goals of modern condensed matter physics is to couple magnetic and electronic properties to develop materials with novel properties, such as high temperature superconductivity, colossal magnetoresistance (CMR) materials, spintronics, and the recently active area of multiferroic materials, heavy fermion materials can be important to help us understand the interaction between magnetic and electronic quantum fluctuations.

The remaining of this paper are organized as follows: In Sec. II we will explain in more detail the mechanisms and physical processes resulting in the unconventional properties of heavy fermion materials, in which the so-called Kondo effect plays the most important role. In Sec. III and Sec. IV we will respectively talk about two important subcategories of heavy fermion systems: Kondo insulators and heavy fermion superconductors.

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II. HEAVY FERMION AND KONDO EFFECT

A. Kondo effect

To understand heavy fermion systems, the first notion we must know is the so-called Kondo effect [3][4]. Loosely speaking, the Kondo effect refers to certain unconventional phenomena result from the process by which a free magnetic impurity ion becomes "screened" by the spins of the Fermi sea at low temperatures and low magnetic fields. As the impurity ion is screened, a portion of conduction electrons are bonded to it and hence the conductivity decreases. However, generally the electronic resistivity due to scattering of conduction electrons by impurities drops monotonically with decreasing temperature. So the two competent mechanisms will lead to a minimal resistivity at low temperatures. This is the explanation, which was given by Kondo in 1963, to the puzzling "minimal conductivity" discovered 30 years before [5].

In the remaining of this subsection, for the convenience of subsequent formulation of heavy fermion physics, we will start from the famous Anderson model, and in a step-by-step manner, finally go to Kondo's idea and results.

In 1961, Anderson [6] gave the first microscopic model for the formation of magnetic moments in metals. Anderson's model Hamiltonian is written as:

$$\begin{aligned} H &= \sum_{k,\mu} \epsilon_k n_{k\mu} + \sum_{k,\mu} V(k)[c^\dagger_{k\mu} f_\mu + f^\dagger_\mu c_{k\mu}] \\ &+ E_f n_f + U n_{f\uparrow} n_{f\downarrow}. \end{aligned} \tag{2}$$

The first and the third term are respectively the Hamiltonian of conduction electrons and that of impurity atom. New insights as well as complications arise from the second and the fourth term. The second term describes the interaction between conduction electrons and the local impurity spin. And the fourth term represents Coulomb interaction between f-electrons at the impurity site.

Anderson model can explain how a localized impurity magnetic moment is formed in the host metal. Once the local moment is formed, another model is introduced to describe the interaction between local spin and conduction electrons. This is the *s*-*d* exchange model, whose Hamiltonian is:

$$H = \sum_{k,\mu} \epsilon_k n_{k\mu} - (\frac{J}{N}) \sum_{k,k'} \sum_{\mu,\mu'} \hat{\boldsymbol{S}} \cdot \hat{\boldsymbol{\sigma}}_{\mu\mu'} c^\dagger_{k\mu} c_{k'\mu'}, \tag{3}$$

which, alternatively, can also be derived from Anderson Hamiltonian by applying the Schrieffer-Wolff transformation [7]. Because the absolute value of the coupling constant J is always much smaller than the Fermi energy of conduction electrons, perturbation techniques can be well adapted. While the first order perturbation theory only gives a temperature independent resistivity, Kondo discovered that the second order perturbation gives a logarithmic dependence of resistivity on temperature:

$$\rho = a - b \ln T, \tag{4}$$

which is just the behavior observed in the temperature range close to the resistivity minimum in dilute magnetic alloys.

The second order perturbation include two virtual processes all called "superexchange", in which an electron or hole is replaced by another conduction counterpart with a different spin. This process can induce an equivalent interaction between conduction electrons and local impurity $d-$ (or$f-$) spins. In most dilute magnetic alloys this induced coupling is antiferromagnetic.

Experiments further showed that when $T \to 0$K, the specific heat of those metals with magnetic impurities deviates dramatically from the law of linear dependence on T in common metals. This is explained as that when $T \to 0$K, magnetic impurities gradually lose their magnetic moments because of the Kondo screening, which will lead to a drop of the impurities' entropy and hence the uncommon behavior of specific heat. So it is natural to expect that the ground state of the system at $T = 0$K is the singlet state between conduction and impurity spins. However, Kondo's perturbation treatment are not suitable at low temperatures. This can be seen from the divergence of the logarithmic temperature dependence of Kondo's result. Thus people must find other ways to strictly prove the existence of Kondo singlet. K. G. Wilson [8] employed the renormalization group method and achieved this goal in 1975. Wilson's treatment is numerical. 5 years later, Andrei [9] and Wiegmann [10], using the Bethe ansatz, gave the strict analytical solution of single impurity Kondo problem.

B. Kondo lattice and heavy fermion system

One characteristic of heavy fermion materials is that every unit cell of the lattice has an ion with localized magnetic moment. Thus a heavy fermion system is just the periodical version of the Kondo system. So it is tempting to construct a periodic Hamiltonian based on the Anderson model:

$$\begin{aligned} H = &\sum_{k,\mu} \epsilon_k n_{k\mu} + \sum_{l,\mu} E_0 n^f_{l\mu} + U \sum_l n^f_{l\uparrow} n^f_{l\downarrow} \\ &+ \frac{V}{\sqrt{N}} \sum_{k,l,\mu} [c^\dagger_{k\mu} f_{l\mu} e^{-i\boldsymbol{k}\cdot\boldsymbol{l}} + f^\dagger_{l\mu} c_{k\mu} e^{i\boldsymbol{k}\cdot\boldsymbol{l}}]. \end{aligned} \tag{5}$$

Models like this are called Anderson Lattice Model. In our model the simplifications include: (1)Neglect the dependence of the strength of s-f hybridization on k, i.e., $V_k = V$. (2)The f states at every site are all nondegenerate. Besides that, the factor $(1/\sqrt{N}) \exp(\pm i\boldsymbol{k} \cdot \boldsymbol{l})$ we introduced in the hybridization term is to reflect the fact that conduction electrons hybridize with the f electron at every site, and every site has a different phase.

When there is no hybridization, at every site there are four eigenstates of f electrons: no electrons(spins) $|0\rangle$, two antiparallel spins $|\uparrow\downarrow\rangle$, and two single spin states $|\uparrow\rangle$ and $|\downarrow\rangle$. Because these four states are orthogonal to each other and complete, we can use them as basis to represent operators $f_{l\mu}$ and $f_{l\mu}^\dagger$:

$$f_\uparrow^\dagger = |\uparrow\rangle\langle 0| + |\uparrow\downarrow\rangle\langle\downarrow|, f_\downarrow^\dagger = |\downarrow\rangle\langle 0| - |\uparrow\downarrow\rangle\langle\uparrow|, \quad (6)$$

and the corresponding formulae for $f_\uparrow$ and $f_\downarrow$ are just their Hermite conjugate. The completeness condition requires

$$|0\rangle\langle 0| + |\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow| + |\uparrow\downarrow\rangle\langle\uparrow\downarrow| = 1. \quad (7)$$

In heavy fermion materials the on-site Coulomb repulsion is always large enough to almost exclude the possibility of double occupancy. So we only need to consider the limit case when $U \to \infty$. The direct result of this limit is that we can simply remove the state $|\uparrow\downarrow\rangle$, and then the f electron operators $f_{l\mu}$ can be expressed using the so-called Hubbard operators $X_{pq}(l) = |lp\rangle\langle lq|$:

$$\begin{aligned} f_{l\mu}^\dagger &= |l\mu\rangle\langle l0| \equiv X_{\mu 0}(l) \\ f_{l\mu} &= |l0\rangle\langle l\mu| \equiv X_{0\mu}(l), \end{aligned} \quad (8)$$

and consequently,

$$n_{l\mu}^f = |l\mu\rangle\langle l\mu| \equiv X_{\mu\mu}(l), \quad (9)$$

and the projection operator to the empty state is define to be $X_{00}(l)$:

$$|l0\rangle\langle l0| \equiv X_{00}(l). \quad (10)$$

With these equations, the Hamiltonian of the Infinite U Anderson Lattice Model is written as

$$\begin{aligned} H &= \sum_{k,\mu} \epsilon_k n_{k\mu} + \sum_{l,\mu} E_0 X_{\mu\mu}(l) \\ &+ \frac{V}{\sqrt{N}} \sum_{k,l,\mu} [c_{k\mu}^\dagger X_{0\mu}(l) e^{-i\boldsymbol{k}\cdot\boldsymbol{l}} + X_{\mu 0}(l) c_{k\mu} e^{i\boldsymbol{k}\cdot\boldsymbol{l}}]. \end{aligned} \quad (11)$$

And the completeness condition Eq. (7) becomes a constraint:

$$X_{00}(l) + X_{\uparrow\uparrow}(l) + X_{\downarrow\downarrow}(l) = 1. \quad (12)$$

However, from Eq. (8) and (12) one can find that the commutation relation of Hubbard operators is neither fermion nor boson's. Thus one cannot directly use the standard Feynman diagram method to calculate this model. To resolve this difficulty, Coleman [12] proposed the "slave boson" technique.

Coleman's idea is to express the Hubbard operators by certain combinations of fermion and boson operators. Let $b_l^\dagger$ and $f_{l\mu}^\dagger$ be standard boson and fermion operators respectively. Coleman wrote down the Hubbard operators X_{00} and $X_{\mu\mu}$ as

$$X_{00}(l) = b_l^\dagger b_l, X_{\mu\mu}(l) = f_{l\mu}^\dagger f_{l\mu}. \quad (13)$$

Thus the constraint (12) becomes

$$b_l^\dagger b_l + f_{l\uparrow}^\dagger f_{l\uparrow} + f_{l\downarrow}^\dagger f_{l\downarrow} = 1. \quad (14)$$

Coleman called the bosons b_l and $b_l^\dagger$ slave bosons. It is easily seen that the number operator of slave bosons determine the probability of unoccupied f electron state at site l, and that of the fermions $f_{l\mu}$ and $f_{l\mu}^\dagger$ represents the probability of single occupation. Furthermore, the hybridization terms are written as

$$X_{\mu 0}(l) = f_{l\mu}^\dagger b_l, X_{0\mu}(l) = f_{l\mu} b_l^\dagger, \quad (15)$$

and it can be shown that these constructions can indeed yield the nonconventional commutators of Hubbard operators.

Using these new operators, Hamiltonian (11) can be rewritten as

$$\begin{aligned} H &= \sum_{k,\mu} \epsilon_k n_{k\mu} + \sum_{l,\mu} E_0 f_{l\mu}^\dagger f_{l\mu} \\ &+ \frac{V}{\sqrt{N}} \sum_{k,l,\mu} [c_{k\mu}^\dagger f_{l\mu} b_l^\dagger e^{-i\boldsymbol{k}\cdot\boldsymbol{l}} + f_{l\mu}^\dagger b_l c_{k\mu} e^{i\boldsymbol{k}\cdot\boldsymbol{l}}]. \end{aligned} \quad (16)$$

Now all the operators in the Hamiltonian are standard fermion or boson operators. So standard perturbation theory based on Wick theorem and Feynman diagram can be applied. However, there is still an obstacle, that is, the constraint (14), which has to be taken into consideration in calculation every Feynman diagram. Coleman noticed that since $[\hat{Q}_l, H] = 0$, one can introduce a time independent field λ_l to include the constraint (14) explicitly through the formula of δ function:

$$\delta_{\hat{Q}_l,1} = \frac{\beta}{2\pi} \int_{-i\pi/\beta}^{i\pi/\beta} e^{-\lambda_l(\hat{Q}_l - 1)} d\lambda_l. \quad (17)$$

Thus the partition function of the infinite U Anderson Lattice Model

$$\begin{aligned} Z &= \mathrm{Tr}_{(\hat{Q}_l=1)}[e^{-\beta H}] \\ &= (\prod_l \int_{-i\pi/\beta}^{i\pi/\beta} \frac{\beta}{2\pi} d\lambda_l) \mathrm{Tr}[e^{-\beta H(\lambda)}], \end{aligned} \quad (18)$$

where

$$\begin{aligned} H(\lambda) &\equiv H + \sum_l \lambda_l (\hat{Q}_l - 1) \\ &= \sum_{k,\mu} \epsilon_k n_{k\mu} + \sum_{l,\mu} E_0 f_{l\mu}^\dagger f_{l\mu} \\ &+ \frac{V}{\sqrt{N}} \sum_{k,l,\mu} (c_{k\mu}^\dagger f_{l\mu} b_l^\dagger e^{-i\boldsymbol{k}\cdot\boldsymbol{l}} + \mathrm{h.c.}) \\ &+ \sum_l \lambda_l (b_l^\dagger b_l + f_{l\uparrow}^\dagger f_{l\uparrow} + f_{l\downarrow}^\dagger f_{l\downarrow} - 1). \end{aligned} \quad (19)$$

Coleman [13] further rewrote the partition function (18) as a path integral and used the saddle-point approximation to calculate the partition function. We will not go

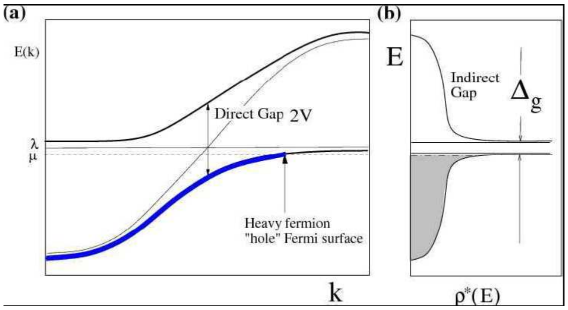

FIG. 2: (a) Dispersion produced by the injection of a composite fermion into the conduction sea.(b) Renormalized density of states, showing "hybridization gap" (Δ_g). [16]

further on this technique. Nevertheless it is worthwhile to mention here that in the degenerate Anderson Lattice Model, where there are degeneracies from orbital degrees of freedom, as in the case of heavy fermion materials containing Ce, Coleman's path integral technique can be combined with another technique called large N expansion, here the N is the number of degeneracy, to give approximate analytical results.

Based on Coleman's slave boson technique, Read and Newns proposed a mean-field theory of infinite U Anderson Lattice Model, which starts from the mean-field approximations:

$$b_l^\dagger \to \langle b_l^\dagger \rangle \equiv r, b_l \to \langle b_l \rangle \equiv r, \lambda_l \to \lambda. \tag{20}$$

This is called the slave boson mean-field approximation (SBMFA). The resulting Hamiltonian from (19)

$$H_{MF} = \sum_{k,\mu} \epsilon_k n_{k\mu} + \sum_{l,\mu} E_f f_{l\mu}^\dagger f_{l\mu} + \frac{V'}{\sqrt{N}} \sum_{k,l,\mu} (c_{k\mu}^\dagger f_{l\mu} e^{-i\boldsymbol{k}\cdot\boldsymbol{l}} + \text{h.c.}) + N\lambda(r^2-1), \tag{21}$$

where $E_f = E_0 + \lambda$, $V' = rV$, is called renormalized hybridized-band model, and can be strictly solved.

The calculated dispersion and density of states from above model is depicted in Fig. 2. From Fig. 2(a) one can see that around the Fermi energy there is an indirect "hybridization gap" of width $\Delta_g \sim T_K$ where T_K is the Kondo temperature. And the direct gap between the upper and lower bands, which are built by hybridized conduction electron and f-electron states, is $2|V|$ where V is the strength of the slave boson field. It should be emphasized here that the gap is solely due to hybridization between conduction and f-electrons and cannot be explained by conventional band theory. Furthermore, in Fig. 2(b) we can see that the density of states near the gap is extremely high, which is due to the contribution of f-electrons. Then from the well-known relation between quasiparticle density of states ρ^* and effective carrier mass m^*:

$$\frac{m^*}{m} = \frac{\rho^*}{\rho}, \tag{22}$$

one can see that it is this unconventional peak of density of states that results in the large effective mass in heavy fermion materials.

TABLE I: Examples of Kondo insulators or semiconductors, with their crystallographic structure and activation gap evaluated from the transport measurements [15].

	Structure	Δ(K)
CeNiSn	ε -TiNiSn	3
$Ce_3Bi_4Pt_3$	$Y_3Sb_4Au_3$	42
SmB_6	CaB_6	27
SmS	NaCl	300-3000
TmTe	NaCl	3500
YbB_{12}	UB_{12}	62
UNiSn	MgAgAs	700
FeSi	FeSi	300

III. KONDO INSULATOR

In experiments, people found that the vast majority of cases the $T = 0$ ground state of heavy fermion materials is metallic, though that may be together with other phases such as paramagnetic, antiferromagnetic or superconducting. However, in a limited number of cases the ground state is insulating with a small energy gap. Table I gives some examples of this class of heavy fermion materials.

Theoretically Kondo insulators are heavy fermion systems in which the lower band in Fig. 2 are filled and the chemical potential lies in the middle of the hybridization gap. One distinctive property of Kondo insulators is that the measured gap is dependent on temperature, which is different from that in conventional semiconductors. This is not hard to understand if considering the fact that at high temperatures heavy fermion materials become regular. Using the renormalized hybridized-band model one can find that approximately the hybridization gap $\Delta \propto r^2$, where r is defined in Eq. (20). Remembering $r^2 \sim \langle b_l^\dagger b_l \rangle = \langle X_{00}(l) \rangle$ is actually the average probability of unoccupation of f states, it must decrease with increasing temperature since f electrons tend to be localized at high temperatures. Thus the gap should also depend on temperature and will disappear at high temperatures.

Another aspect worth noting is that, in many Kondo insulators, the gap is very small (~meV), and can be easily tuned by pressure, external field and doping. For further details the reader can refer to, for example, the review by Riseborough [17].

IV. HEAVY FERMION SUPERCONDUCTIVITY

Since superconductivity is another huge regime that would require dozens of pages of background introduction, the purpose of this section is just to introduce basic experimental discoveries in heavy fermion superconductivity, and some ideas in the theory side.

In the framework of BCS theory, magnetic impurities in a metal will strongly destroy the superconductivity since its interaction with two electrons in a spin singlet state will break the pairing. However, because electrons in heavy fermion materials lose their magnetic moments at low temperatures and become fermi liquid again, it is reasonable to suppose that superconductivity may arise in certain heavy fermion systems.

This is indeed the case. Since the first discovery of superconductivity in $CeCu_2Si_2$ by Steglich et al. [18], the list of known heavy fermion superconductors has grown to include more than a dozen materials with a great diversity of properties. They include:

(1) "Canonical" heavy fermion superconductors, such as $CeCu_2Si_2$ and UPt_3. They develop superconductivity out of a paramagnetic Landau Fermi liquid.

(2) "Pre-ordered" superconductors, such as UPt_2Al_3, $CePt_3Si$ and URu_2Si_2. They develop another order before superconductivity emerging at a lower temperature. For example, in UPt_2Al_3 and $CePt_3Si$ there is an antiferromagnetic phase before the system going to the superconducting phase.

(3) "Quantum critical" superconductors, such as $CeIn_3$ and $CeCu_2(Si_{1-x}Ge_x)_2$. In these materials superconductivity arises only when pressure are tuned close to a quantum critical point.

(4) "Strange" superconductors, including UBe_{13}, $CeCoIn_5$ and $PuCoGa_5$. In these materials the superconducting state emerges out of some strange non-Fermi-liquid state. For example, $PuCoGa_5$ transitions directly from a Curie paramagnet of unquenched f-spins into a superconductor.

On top of this classification, there are also many common features of heavy fermion superconductors. One of them is the large value of the electronic specific heat coefficient (C_p/T) at T_c (Fig. 3), which indicates the heavy quasiparticles participate in the superconducting pairing. Another confirmation of the "heavy" nature of the pairing electrons comes from observed penetration depth λ_L and superconducting coherence length ξ. The large mass of the quasiparticles enhances the penetration depth while decreasing the coherence length.

From these common properties, it is straightforward to assume a Fermi liquid of itinerant heavy electrons, which is an electronic analog of superfluid He_3, in which the quasiparticles interact through a phenomenological BCS model. Thus for most purposes, Landau-Ginzburg theory is sufficient. However, this is not applicable in the case of the 4th category superconductors mentioned above, where a microscopic theory is required to take the formation of heavy quasiparticles into consideration from the beginning. However this is a hard work comparable with the microscopic model of high-T_c superconductivity, and has not been thoroughly addressed yet. For more information on the theory of heavy fermion superconductors

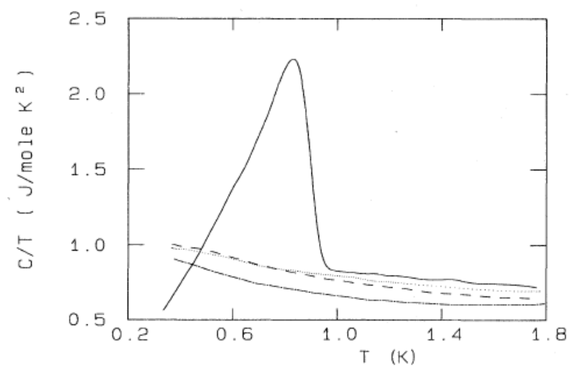

FIG. 3: Specific heat divided by temperature vs. temperature for UBe_{13} in applied magnetic fields of 0 (solid), 9 (dotted), 15 (dashed), and 20 (dot-dashed) T. [19]

one can refer to [16].

In conclusion, this is a very insufficient review on this huge, long-studied, but still active area, which is also one of the most challenging subjects in solid state physics. The study of heavy fermions has inspired the idea of composite fermions, high-T_c superconductivity and many other important subjects. And both experimentalists and theorists are still keeping revealing novel phenomena and new understandings in this field. To get a comprehensive knowledge on heavy fermion physics we suggest the reader to refer to those excellent reviews and books such as [16],[20] and [21].

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