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## Normal-state properties of heavy-fermion systems with conduction-band impurities

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**Abstract.** The effects of conduction-band (CB) impurities in heavy-fermion systems are studied on the basis of the  $U \rightarrow \infty$  periodic Anderson model in the framework of a slave-boson mean-field theory within the single-site coherent-potential approximation (CPA). We provide a simplified CPA formalism for the treatment of mixing disorder induced by CB alloying. The density of states for conduction and localized f electrons can be calculated self-consistently in the whole impurity-concentration range. The concentration dependence of the specific-heat coefficient, static magnetic susceptibility and resistivity at low temperatures as well as the Kondo temperature in the alloys is obtained. The results indicate that the experimental observations in  $\text{CeCu}_6$  upon doping with Au, Ag and Al can be qualitatively explained as the effects of mixing disorder.

### 1. Introduction

The heavy-fermion (HF) systems, with a very large density of states (DOS) at the Fermi level, contain an entire class of rare-earth or actinide intermetallic compounds. Some of them which show neither magnetic nor superconducting order at extremely low temperatures may be described in terms of a Fermi liquid with a very large effective mass [1, 2]. Recently, however, many experimental observations show a weak stability of the normal phase of HF systems [3–5], and the conventional Fermi-liquid picture is facing a challenge. In order for the nature of normal HF materials including the proximity to magnetism to be understood more thoroughly, much attention has been in the past few years to the effects of alloying, especially with conduction-band (CB) impurities. Many pieces of evidence reveal a strong impurity-concentration dependence of physical properties of these alloys [6–11]. In  $\text{CeCu}_6$ , for example, accompanying the expansion in cell volume induced by substitutions of Au or Ag on Cu sites, the specific-heat coefficient  $\gamma$  and the magnetic susceptibility  $\chi$  increase with increasing CB impurities, and the magnetic order is established in the ground state, whereas Al substitutions for Cu decrease the cell volume and result in the reduction of  $\gamma$  and  $\chi$ ; moreover fairly dilute Al impurities can also lead to the suppression of the low-temperature resistivity peak of  $\text{CeCu}_6$ . All these phenomena provide some important information for the exploration of the microscopic origin of the weak stability of normal phase, and the theoretical study of the CB-alloying effects is significant in the systematic understanding of the normal-state properties of HF systems.

The elucidation of the low-temperature properties with CB impurities demands a self-consistent alloy theory applicable to the case of finite temperature and over the whole impurity concentration range ( $0 \leq c \leq 1$ ). Theoretically, progress has been made in the study of the HF alloys. Within the single-site coherent-potential approximation (CPA), a

Kondo-alloy theory proposed by Xu and Li has successfully handled the drastic disorder on the bare f level due to Kondo holes [12, 13]. However, as for the CB impurities, they have no direct influence on the bare f level since the substitutions occur at non-f metal atoms. Apparently, their main effects are quite different from those of Kondo holes. An anomalously large electronic Grüneisen constant [14] and a dramatic variation of Kondo temperature with an applied pressure [15, 16] have been detected from experiments on HF systems. All these indicate that the mixing strength is sensitive to the variation in cell volume, and the change in c–f mixing strength may be significant even though the cell-volume change due to the CB impurity is small. On the other hand, some theoretical investigations [17–19] have proved that the potential disorder in the conduction-electron energies has a weak influence on the coherence of HF systems, and it is negligible in comparison with the drastic effect of mixing disorder. Therefore, we may describe the CB-doped HF systems by introducing only the mixing disorder into the periodic Anderson model (PAM). Some research works based on this disorder model have successfully explained the experimental results concerning the magnetic instability and residual magneto-resistivity of HF systems with CB impurities [20–22]. The purpose of this paper is to establish a simplified CPA theory for the HF alloy with CB impurities in the framework of the slave-boson (SB) mean-field approximation (MFA). We expect to give a unified explanation of alloying effects, including the concentration dependence of the DOS, Kondo temperature  $T_K$ , specific-heat coefficient  $\gamma$ , static magnetic susceptibility  $\chi$  and resistivity  $\rho$ .

The rest of this paper is organized as follows. We shall describe the disorder model with CB impurities in the SBMFA in section 2, and introduce a simplified CPA formalism in section 3. In section 4, the variation of Kondo temperature and DOS induced by impurities will be discussed, and an attempt to explain the effect of the CB impurities on low-temperature thermodynamic and transport properties will be shown. Finally, our results will be summarized in section 5.

## 2. Disorder model of HF alloys with CB impurities

The  $U \rightarrow \infty$  PAM is referred to as a suitable description for the normal state of HF metals [23, 24]. With the aid of the SB technique introduced by Barnes [25] and Coleman [26], the strong on-site correlation between f electrons is clearly described, and the Hamiltonian becomes easily solvable in the MFA giving rise to exact results in the large-degeneracy limit, from which a Fermi liquid state with large effective mass is obtained [23]. When the system is doped with conduction-band impurities, as discussed in section 1, the main effect, that the impurities can bring about a local change in the cell volume thus give rise to a change in the c–f mixing strength at the impurity sites, should be considered. The Hamiltonian of the HF alloy can then be written as

$$H = \sum_{k\sigma} \epsilon_k c_{k\sigma}^+ c_{k\sigma} + \sum_{l\sigma} (V + \xi_l \Delta V) (c_{l\sigma}^+ b_l^+ f_{l\sigma} + f_{l\sigma}^+ b_l c_{l\sigma}) + \sum_{l\sigma} E_0 f_{l\sigma}^+ f_{l\sigma} \quad (1)$$

with a constraint reflecting the strong on-site f–f correlation

$$\sum_{\sigma} f_{l\sigma}^+ f_{l\sigma} + b_l^+ b_l = 1 \quad (2)$$

where  $c_{k\sigma}^+$  ( $f_{l\sigma}$ ) is the creation (annihilation) operator of the conduction (localized) electron in the Bloch (Wannier) state labelled by momentum  $\mathbf{k}$  (site  $l$ ) and spin  $\sigma$ ;  $\xi_l$  is the random variable with  $\xi_l = 0$  for a site  $l$  with no impurities and  $\xi_l = 1$  for a CB-impurity-occupied site  $l$ , where the c–f mixing strength  $V$  changes by  $\Delta V$ . Note that the random average  $\overline{\xi_l^2} = \overline{\xi_l} = c$ , where  $c$  is the normalized concentration of CB impurities.

In the MFA, both  $b_l$  and  $b_l^+$  can be replaced by a c-number  $r$ , and a Lagrange multiplier  $\lambda$  is introduced to ensure the satisfaction of the constraint (2). Then the MFA Hamiltonian is reduced to

$$\tilde{H} = \sum_{k\sigma} (c_{k\sigma}^+, f_{k\sigma}^+) \mathcal{E}_k \begin{pmatrix} c_{k\sigma} \\ f_{k\sigma} \end{pmatrix} + \sum_{l\sigma} \xi_l (c_{l\sigma}^+, f_{l\sigma}^+) \Delta\mathcal{V} \begin{pmatrix} c_{l\sigma} \\ f_{l\sigma} \end{pmatrix} + N\lambda(r^2 - 1) \quad (3)$$

with

$$\mathcal{E}_k \equiv \begin{pmatrix} \epsilon_k & rV \\ rV & E_f \end{pmatrix} \quad (4)$$

and

$$\Delta\mathcal{V} \equiv \begin{pmatrix} 0 & r\Delta V \\ r\Delta V & 0 \end{pmatrix} \quad (5)$$

where the renormalized f level is defined as  $E_f \equiv E_0 + \lambda$ , and  $N$  is the number of lattice sites. The SB parameters  $r$  and  $\lambda$  are determined by the minimum condition of the free energy

$$\sum_{\sigma} \langle f_{l\sigma}^+ f_{l\sigma} \rangle = 1 - r^2 \quad (6)$$

$$(V + \xi_l \Delta V) \sum_{\sigma} \langle c_{l\sigma}^+ f_{l\sigma} + f_{l\sigma}^+ c_{l\sigma} \rangle + 2r\lambda = 0. \quad (7)$$

The appearance of the random variable  $\xi_l$  in (3) and (7) implies that the standard procedure is unable to diagonalize the disordered Hamiltonian. Therefore, we shall adopt the single-site CPA to solve this disordered model self-consistently.

### 3. Mixing renormalization in CPA regime

The idea of the CPA is to replace the disorder potential of impurities  $\xi_l \Delta\mathcal{V}$  by a translationally invariant but energy-dependent coherent potential of the effective medium

$$\mathcal{S}(\omega) \equiv \begin{pmatrix} S_{cc}(\omega) & S_{cf}(\omega) \\ S_{fc}(\omega) & S_{ff}(\omega) \end{pmatrix} \quad (8)$$

as embodied in the effective Hamiltonian

$$\tilde{H} = \sum_{k\sigma} (c_{k\sigma}^+, f_{k\sigma}^+) [\mathcal{E}_k + \mathcal{S}(\omega)] \begin{pmatrix} c_{k\sigma} \\ f_{k\sigma} \end{pmatrix} + N\lambda(r^2 - 1) \quad (9)$$

from which the matrix of medium Green's function (GF) in the space of basis vectors  $(c_{k\sigma}, f_{k\sigma})^T$

$$\mathcal{G}(\mathbf{k}, \omega) \equiv \begin{pmatrix} G_{cc}(\mathbf{k}, \omega) & G_{cf}(\mathbf{k}, \omega) \\ G_{fc}(\mathbf{k}, \omega) & G_{ff}(\mathbf{k}, \omega) \end{pmatrix} = [\omega - \mathcal{E}_k - \mathcal{S}(\omega)]^{-1} \quad (10)$$

is derived. The determination of  $\mathcal{S}(\omega)$  is related to a self-consistent requirement of the CPA. In the single-site CPA, the potential  $\mathcal{S}(\omega)$  has to be determined in such a way that in the effective medium the average relative scattering by impurities vanishes at each site [27]. According to [27], this condition is equivalent to a self-consistent equation

$$\mathcal{S}[1 - \mathcal{F}(\Delta\mathcal{V} - \mathcal{S})] = c \Delta\mathcal{V} \quad (11)$$

with the averaged site GF of the effective medium

$$\mathcal{F}(\omega) \equiv \begin{pmatrix} F_{cc}(\omega) & F_{cf}(\omega) \\ F_{fc}(\omega) & F_{ff}(\omega) \end{pmatrix} = N^{-1} \sum_{\mathbf{k}} \mathcal{G}(\mathbf{k}, \omega) \quad (12)$$

which has the matrix-element expression

$$F_{cc} = N^{-1} \sum_k \left[ \omega - \epsilon_k - S_{cc} - \frac{(rV + S_{cf})(rV + S_{fc})}{\omega - E_f - S_{ff}} \right]^{-1} \quad (13)$$

$$F_{cf} = F_{cc} \frac{rV + S_{cf}}{\omega - E_f - S_{ff}} \quad (14)$$

$$F_{fc} = \frac{rV + S_{fc}}{\omega - E_f - S_{ff}} F_{cc} \quad (15)$$

$$F_{ff} = \frac{1}{\omega - E_f - S_{ff}} \left[ 1 + \frac{(rV + S_{fc})F_{cc}(rV + S_{cf})}{\omega - E_f - S_{ff}} \right]. \quad (16)$$

In general, it is difficult to solve the nonlinear equation (11) self-consistently. Noting that there exists only mixing disorder in our model, we can introduce the renormalized mixing term  $\overline{V^2}(\omega)$  with the definition

$$\frac{r^2 \overline{V^2}}{\omega - E_f} \equiv S_{cc} + \frac{(rV + S_{cf})(rV + S_{fc})}{\omega - E_f - S_{ff}} \quad (17)$$

to reflect the alloying effects so that the CPA formalism may be simplified (the details will be given in the appendix). After some algebraic manipulations of (11) with the use of (13)–(17), the self-consistent CPA equation can be simplified as

$$\frac{c}{\overline{V^2} - V^2} + \frac{1 - c}{\overline{V^2} - (V + \Delta V)^2} + \frac{r^2 F_{cc}(\omega)}{\omega - E_f} = 0 \quad (18)$$

which naturally reduces to the lattice case

$$\overline{V^2} = \begin{cases} V^2 & c = 0 \\ (V + \Delta V)^2 & c = 1 \end{cases} \quad (19)$$

and has a more compact form

$$F_{cc}(\omega) = \frac{c}{\Sigma_{cc}(\omega, 0) - \Sigma_{cc}(\omega, c)} + \frac{1 - c}{\Sigma_{cc}(\omega, 1) - \Sigma_{cc}(\omega, c)} \quad (20)$$

in terms of the self-energy of conduction electrons  $\Sigma_{cc}(\omega, c) \equiv r^2 \overline{V^2} / (\omega - E_f)$  in the effective medium. In the meantime, the relation

$$\frac{rV + S_{cf}}{\omega - E_f - S_{ff}} = \frac{rV + S_{fc}}{\omega - E_f - S_{ff}} = \frac{r[\overline{V^2} + V(V + \Delta V)]}{(\omega - E_f)[V + (V + \Delta V)]} \quad (21)$$

is obtained. Therefore, we can define

$$\overline{V} \equiv \frac{\overline{V^2} + V(V + \Delta V)}{V + (V + \Delta V)} \quad (22)$$

so that the matrix elements of the site GF can be expressed in analogy with the lattice case as

$$F_{cc} = N^{-1} \sum_k \left[ \omega - \epsilon_k - \frac{r^2 \overline{V^2}}{\omega - E_f} \right]^{-1} \quad (23)$$

$$F_{cf} = F_{fc} = \frac{r \overline{V}}{\omega - E_f} F_{cc} \quad (24)$$

$$F_{ff} = \frac{1}{\omega - E_f} \left[ 1 + \frac{r^2 \overline{V^2}}{\omega - E_f} F_{cc} \right]. \quad (25)$$

In the alloy case ( $0 < c < 1$ ),  $\bar{V}^2$  is generally the complex number with the small imaginary part leading to a finite lifetime of heavy fermions.

Now, in combination with the CPA equation (18), definition (22) and expressions of GF (23)–(25), the SB parameters  $r$  and  $\lambda$  can be determined self-consistently. In the effective medium, the SB equations (6) and (7) may be rewritten by taking an average over the randomness and using GF spectral theorem as

$$1 - r^2 = -\frac{2}{\pi} \int_{-\infty}^{+\infty} d\omega f(\omega - \mu) \text{Im} F_{\text{ff}}(\omega + i0^+) \quad (26)$$

$$r\lambda = \frac{2(V + c\Delta V)}{\pi} \int_{-\infty}^{+\infty} d\omega f(\omega - \mu) \text{Im} F_{\text{cf}}(\omega + i0^+) \quad (27)$$

where  $f(\omega - \mu)$  is the Fermi distribution function and (23) has been made use of. The chemical potential  $\mu$  is determined by the total number of electrons

$$n_c + 1 = -\frac{2}{\pi} \int_{-\infty}^{+\infty} d\omega f(\omega - \mu) [\text{Im} F_{\text{cc}}(\omega + i0^+) + \text{Im} F_{\text{ff}}(\omega + i0^+)] \quad (28)$$

where  $n_c$  is the unperturbed conduction electron number per site.

Equations (18) and (22)–(28) constitute a fundamental system of equations for determining the SB parameters and GF of the effective medium. It naturally provides a smooth interpolation between two limits  $c = 0$  and  $c = 1$ , then can easily be applied to calculate the Kondo temperature and electronic DOS of HF alloys with arbitrary CB-impurity concentration.

#### 4. Alloying effects in normal HF systems

We now turn to discuss the CB-alloying effects on the properties of normal HF systems. We have discussed the dependence of  $T_K$  upon the impurity concentration  $c$ . On the basis of the above CPA theory, the zero-temperature electronic DOS and residual resistivity  $\rho_R$  as well as the specific-heat coefficient  $\gamma$ , magnetic susceptibility  $\chi$  and resistivity  $\rho$  at low temperature have been calculated. In these calculations, we take  $E_0 = -0.9 D$ ,  $V = 0.2 D$  and  $n_c = 0.5$ . For simplicity, the DOS of the unperturbed conduction electron is assumed to be a constant with a band width  $2 D$ . The analytic and numerical results which can be compared with the experimental observations [6–11] are shown as follows.

##### 4.1. The Kondo temperature $T_K$

As a signal for transition between the independent magnetic-ion state and the coherent Kondo-lattice state, the Kondo temperature can be determined with the condition  $r = 0$ . After the  $r^2$  terms in (18), (23) and (25) are neglected, equations (26) and (28) give

$$E_f = \mu \approx (n_c - 1)D \quad (29)$$

for  $k_B T_K \ll D$ , and a virtual crystal solution of  $\bar{V}$

$$\bar{V} = (1 - c)V + c(V + \Delta V) \quad (30)$$

can be found from (18) and (22). Substituting (24), (29) and (30) into (27), we arrive at

$$\frac{2(V + c\Delta V)^2}{\pi N(\mu - E_0)} \sum_{\mathbf{k}} \int_{-\infty}^{+\infty} d\omega f_{\mathbf{k}}(\omega - \mu) \text{Im} \left[ \frac{1}{(\omega + i0^+ - \epsilon_{\mathbf{k}})(\omega + i0^+ - \mu)} \right] = 1 \quad (31)$$

with the Fermi function  $f_K(\omega - \mu)$  at  $T_K$ , and can perform the sum and integral to obtain

$$k_B T_K(c) = \frac{2e^\gamma}{\pi} \sqrt{n_c(2-n_c)} D \exp \left\{ -\frac{D[(n_c-1)D - E_0]}{(V + c\Delta V)^2} \right\} \quad (32)$$

which is linearly approximated to

$$T_K(c) = T_K(0) \left\{ 1 + \frac{2D[(n_c-1)D - E_0]\Delta V}{V^3} c \right\} \quad (33)$$

in the dilute limit.

Equations (32) and (33) indicate that the Kondo temperature  $T_K$  increases or decreases monotonically with the impurity concentration  $c$  if the impurities tend to increase or decrease with mixing strength.

Furthermore, the cell-volume dependence of mixing strength can be discussed in terms of  $T_K$ . The CB doping will change the mixing strength dramatically because of the variation of cell volume in the HF system. Experimentally, an anomalously large electronic Grüneisen constant  $\Gamma$  of the order of  $10^2$  has been detected [14], and  $\Gamma$  can be defined as

$$\Gamma \equiv -\frac{\partial \ln T_K}{\partial \ln \Omega} \quad (34)$$

where  $\Omega$  denotes the cell volume. From (32) and (34), the relationship

$$\Delta V = \left\{ \frac{1}{V^2} + \frac{\Gamma}{D[(n_c-1)D - E_0]} \left( \frac{\Delta \Omega}{\Omega} \right) \right\}^{-1/2} - V \quad (35)$$

is attained. It predicts the increase and decrease of mixing strength respectively corresponding to the contraction and expansion of cell observed in experiments for CeCu<sub>6</sub>.

In conclusion, the Kondo coherence of HF systems is affected by CB alloying, as manifested by the variation of the Kondo temperature  $T_K$  in connection with the change in cell volume. In CeCu<sub>6</sub>, Au or Ag substitutions for Cu, with the cell volume increasing and the mixing weakened, drop  $T_K$  and suppress the Kondo coherent state; in contrast, Al substitutions raise  $T_K$  and support the Kondo coherent state.

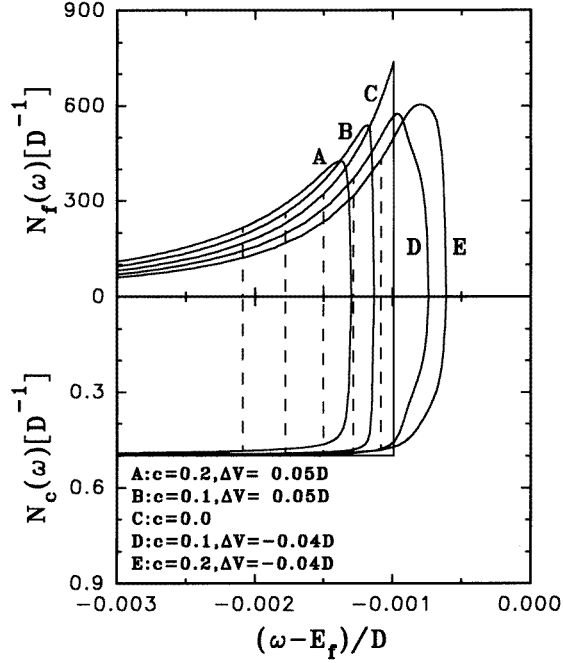
#### 4.2. The electronic DOS at $T = 0$

The electronic DOS is defined by the imaginary part of the site GF. The DOS of conduction and f electrons for each spin can be written as

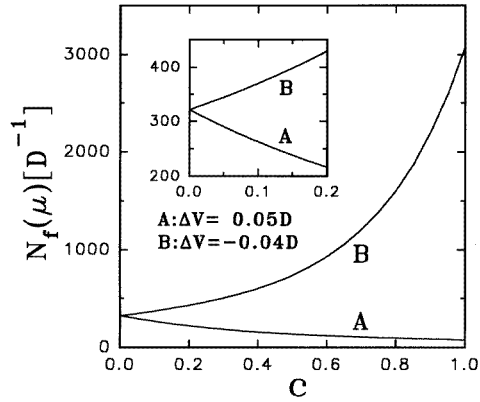
$$N_{c(f)}(\omega) = -\frac{1}{\pi} \text{Im} F_{cc(ff)}(\omega + i0^+) \quad (36)$$

where  $F_{cc}$  and  $F_{ff}$  should be calculated self-consistently from equations (18) and (22)–(28). Although the DOS can be solved analytically in the case of  $c = 0$  and  $c = 1$ , we have to proceed with a numerical calculation in the region of  $0 < c < 1$ .

The numerical results for the DOS near the Fermi level  $\mu$  and  $c$ -dependent f DOS on the Fermi level at  $T = 0$  are respectively shown in figures 1 and 2. In the vicinity of  $\mu$ , the HF systems have the f DOS much larger than the c DOS, and the f DOS is shown to increase with  $c$  if the impurities expand the cell and thus reduce the mixing strength, and to decrease with  $c$  for the opposite condition. With the DOS information, the thermodynamic properties can be naturally explained.



**Figure 1.** The zero-temperature electronic DOS of CB-doped alloys near the Fermi level (denoted by dotted lines).



**Figure 2.** The zero-temperature f DOS of CB-doped alloys at the Fermi level; inset, dilute doping cases.

#### 4.3. The specific-heat coefficient $\gamma$

In the low-temperature region, the main contribution to the specific heat originates from f electrons near the Fermi level because  $N_f(\omega) \gg N_c(\omega)$ ; then the specific-heat coefficient of alloys can be written in terms of the f DOS as

$$\gamma(T) = \frac{1}{2} k_B^2 \beta^3 \int_{-\infty}^{+\infty} d\omega (\omega - \mu)^2 \operatorname{sech}^2 \left[ \frac{\beta(\omega - \mu)}{2} \right] N_f(\omega)$$

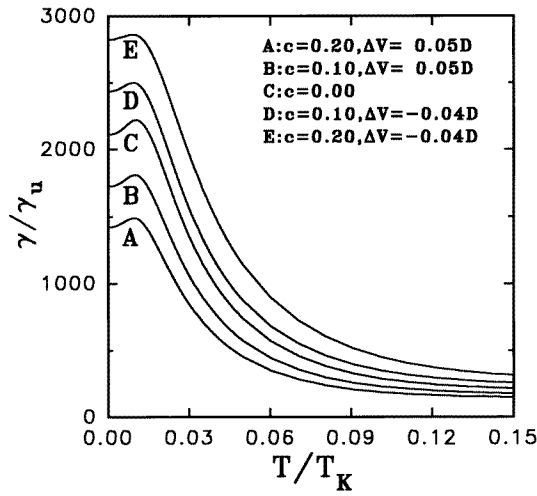


$$= \frac{1}{2} k_B^2 \int_{-\infty}^{+\infty} d\eta \eta^2 \operatorname{sech}^2 \frac{\eta}{2} N_f(\mu + \eta k_B T) \quad (37)$$

with  $\beta = (k_B T)^{-1}$ . At zero temperature, we have

$$\gamma(0) = \frac{2}{3} \pi^2 k_B^2 N_f(\mu). \quad (38)$$

Thus, the zero-temperature specific-heat coefficient is proportional to the f DOS at the Fermi level. Its variation with  $c$  can be illustrated by figure 2. At low temperatures, it can be expected that the shape of the f DOS changes very little in comparison with the zero-temperature case. Then figure 1 is capable of explaining the numerical results of the  $\gamma$ - $T$  curves for various CB-impurity concentrations given in figure 3, which are qualitatively in agreement with experiments [6, 7, 9, 10]. Since the f DOS close to the Fermi level increases or decreases with decreasing or increasing mixing strength, the expansion or contraction of the cell induced by CB impurities will lead to a rise or fall of low-temperature specific-heat coefficient dependent on the concentration, as shown in figure 3.



**Figure 3.** The specific-heat coefficient of CB-doped alloys with  $\gamma_u \equiv k_B^2/D$ .

#### 4.4. The magnetic susceptibility $\chi$

The static magnetic susceptibility for f electrons in HF systems can be expressed in terms of the f DOS as

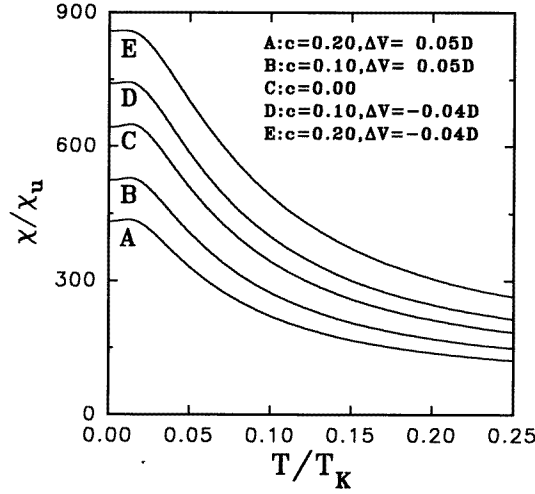
$$\begin{aligned} \chi(T) &= \frac{1}{2} \mu_B^2 \beta \int_{-\infty}^{+\infty} d\omega \operatorname{sech}^2 \left[ \frac{\beta(\omega - \mu)}{2} \right] N_f(\omega) \\ &= \frac{1}{2} \mu_B^2 \int_{-\infty}^{+\infty} d\eta \operatorname{sech}^2 \frac{\eta}{2} N_f(\mu + \eta k_B T) \end{aligned} \quad (39)$$

where  $\mu_B$  is the Bohr magneton. The zero-temperature magnetic susceptibility

$$\chi(0) = 2\mu_B^2 N_f(\mu) \quad (40)$$

is only determined by the f DOS at the Fermi level, so its dependence on  $c$  can also be explained by figure 2. For the same reason as mentioned in subsection 4.3, the variation of low-temperature susceptibility with the impurity concentration can be interpreted in terms of

the change in mixing strength. In accordance with the experiments [6, 7, 10], our numerical results at low temperature sketched in figure 4 display the increase and decrease of  $\chi$  respectively corresponding to negative and positive  $\Delta V$ . The former foreshadows the onset of magnetic order in the ground state (see [20]), and the latter implies the more stable paramagnetic state of HF systems with the mixing strengthened. It is the change in mixing strength that not only results in the variation of the low-temperature magnetic susceptibility with the CB-impurity concentration, but also affects the stability of normal states in HF systems.



**Figure 4.** The magnetic susceptibility of CB-doped alloys with  $\chi_u \equiv \mu_B^2/D$ .

#### 4.5. The resistivity $\rho$

In a perfect Kondo lattice, there should be, in the MFA, no resistivity because of the infinite lifetime of heavy fermions. The non-zero resistivity at finite temperature comes from the charge fluctuations around the MFA [24]. Experimentally and theoretically [1, 24, 28], a Kondo coherence peak at temperature below  $T_K$  and the Fermi-liquid law characterized by the resistivity fall in the form of  $T^2$  after reaching that peak have been confirmed.

When doped with CB impurities, besides the fluctuation-induced resistivity  $\rho_F$ , the HF system will have in the MFA an impurity-scattering resistivity  $\rho_I$  due to the finite lifetime of heavy fermions resulting from the mixing disorder. Its reciprocal, i.e. the conductivity, can be expressed in the Kubo–Greenwood formula

$$\sigma_1(T) = \frac{2\hbar e^2 v_F^2}{3\pi N\Omega} \int_{-\infty}^{+\infty} d\omega \left[ -\frac{\partial f(\omega - \mu)}{\partial \omega} \right] \sum_{\mathbf{k}} [\text{Im } G_{cc}(\mathbf{k}, \omega + i0^+)]^2 \quad (41)$$

with the Fermi velocity  $v_F$ . The appearance of the matrix element of GF  $\mathcal{G}$  in (41) means that the scattering resistivity originates from the imaginary part of the self-energy  $\Sigma_{cc}$  of  $c$  electrons. At a temperature much lower than  $T_K$ , in view of the Fermi-liquid behaviour of  $\rho_F$  [24], we express the total resistivity as

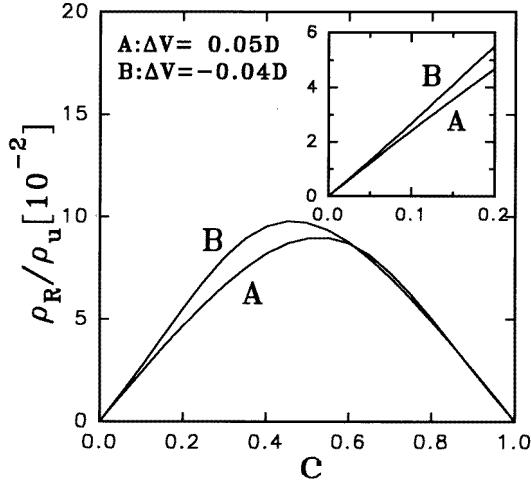
$$\rho(T) = \rho_I(T) + \alpha \left( \frac{T}{T_K} \right)^2 \rho_u \quad (42)$$

where a unit resistivity is defined as  $\rho_u \equiv 3\pi\Omega D^2/2\hbar e^2 v_F^2$  and a suitable dimensionless constant is denoted by  $\alpha$ .

From (42), a residual resistivity only contributed to by the impurity scattering can be found. It can be calculated from the reduced form of (41) at zero temperature

$$\sigma_1(0) = \frac{D^2}{N\rho_u} \sum_k [\text{Im} G_{cc}(k, \mu + i0^+)]^2. \quad (43)$$

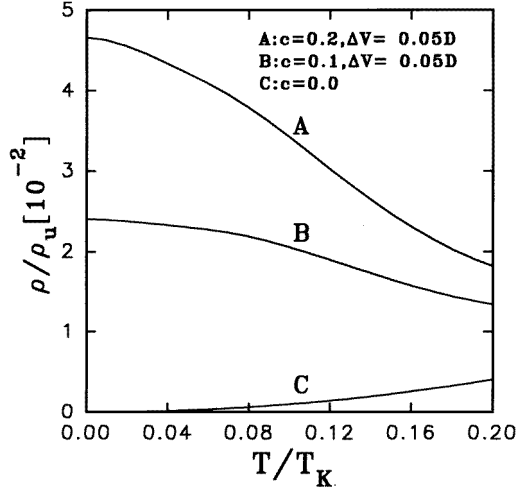
Figure 5 sketches the  $\rho_R$ - $c$  curve, where  $\rho_R = 1/\sigma_1(0)$ . In the low-temperature region, however, both fluctuations and impurity scattering are responsible for resistivity. Apparently, when the system is cooled, the fluctuation resistivity falls, but the scattering resistivity of impurities rises because the imaginary part of  $\Sigma_{cc}$  is proportional to the SB parameter  $r^2$ , which increases with decreasing temperature. Hence how the low-temperature resistivity varies with  $T$  depends on the competition between these two effects. For the dilute doping, increasing the impurity concentration makes the rise of scattering resistivity more sensitive to the increase in  $r^2$ . In a real HF metal such as CeCu<sub>6</sub> with a suitable doping of Al impurities, the rise of  $\rho_I$  with decreasing  $T$  will be rapid enough to overwhelm the fall of  $\rho_F$ , thus the total resistivity increases monotonically with decreasing temperature and the coherence peak vanishes. The relevant numerical results are shown in figure 6, which can be compared with experiments [10, 11].



**Figure 5.** The residual resistivity of CB-doped alloys with  $\rho_u \equiv 3\pi\Omega D^2/2\hbar e^2 v_F^2$ ; inset, dilute doping cases.

## 5. Conclusions

In this paper, we introduced mixing disorder into the Anderson lattice model as a starting point to discuss the CB doping in a HF metal. A mixing-renormalization method based on the single-site CPA theory has been presented under the scheme of SBMFA to describe the alloying effects in the normal state. In this picture, the impurity-concentration dependence of low-temperature properties of normal HF alloys can be explained as a renormalization effect of the mixing. In fact, the real part of the renormalized mixing term, as an interpolating function about the impurity concentration, reflects the effective mixing correlation. Its



**Figure 6.** The resistivity of CB-doped alloys with  $\rho_u \equiv 3\pi\Omega D^2/2\hbar e^2 v_f^2$ .

variation with the concentration leads to a change in the effective mass of heavy fermions near the Fermi level and, in consequence, modifies the thermodynamic properties of HF systems. It may be owing to the increase or decrease in the effective mixing strength that Al or Au and Ag substitutions for Cu in CeCu<sub>6</sub> bring about the fall or rise of the specific-heat coefficient and magnetic susceptibility. On the other hand, the imaginary part of the renormalized mixing term determines a finite lifetime of heavy fermions, and hence affects dramatically the transport properties. For CeCu<sub>6</sub> with Al doping the mixing disorder results in an impurity-scattering resistivity. Its increase with a drop in the temperature suppresses the fall of low-temperature resistivity, then, at a moderate impurity concentration, leads to a monotonic increase of total resistivity and the disappearance of the Kondo coherence peak.

Finally, we would like to point out that the above discussion is valid only for the systems at low temperature. In order to extend our theory to study the properties of the CB-doped HF systems at elevated temperatures, we have to go beyond the MFA. This problem is under investigation.

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### Appendix

Now, we want to give the major steps towards the simplification of CPA formalism. First, we rewrite the CPA equation (11) as

$$U \equiv \mathcal{S}[1 - \mathcal{F}(\Delta\mathcal{V} - \mathcal{S})] - c\Delta\mathcal{V} = 0. \quad (\text{A1})$$

Introducing two-component vectors  $\mathbf{a} \equiv (1, rV/(\omega - E_f))^T$ ,  $\mathbf{b} \equiv (1, r(V + \Delta V)/(\omega - E_f))^T$  and  $\mathbf{c} \equiv (0, 1)^T$  and making use of (14)–(17), we achieve

$$\left( \frac{r^2\overline{V^2}}{\omega - E_f} - \frac{r^2V^2}{\omega - E_f} \right) F_{cc}(\omega) \left[ \frac{r^2\overline{V^2}}{\omega - E_f} - \frac{r^2(V + \Delta V)^2}{\omega - E_f} \right]$$

$$= -(1-c) \left( \frac{r^2 \bar{V}^2}{\omega - E_f} - \frac{r^2 V^2}{\omega - E_f} \right) - c \left[ \frac{r^2 \bar{V}^2}{\omega - E_f} - \frac{r^2 (V + \Delta V)^2}{\omega - E_f} \right] \quad (\text{A2})$$

from  $\mathbf{a}^T \mathcal{U} \mathbf{b} = 0$ ,

$$\begin{aligned} & \left( \frac{r^2 \bar{V}^2}{\omega - E_f} - \frac{r^2 V^2}{\omega - E_f} \right) F_{cc}(\omega) \left[ \frac{rV + S_{cf}}{\omega - E_f - S_{ff}} - \frac{r(V + \Delta V)}{\omega - E_f} \right] \\ &= -(1-c) \left( \frac{rV + S_{cf}}{\omega - E_f - S_{ff}} - \frac{rV}{\omega - E_f} \right) \\ & \quad - c \left[ \frac{rV + S_{cf}}{\omega - E_f - S_{ff}} - \frac{r(V + \Delta V)}{\omega - E_f} \right] \end{aligned} \quad (\text{A3})$$

from  $\mathbf{a}^T \mathcal{U} \mathbf{c} = 0$ ,

$$\begin{aligned} & \left( \frac{rV + S_{fc}}{\omega - E_f - S_{ff}} - \frac{rV}{\omega - E_f} \right) F_{cc}(\omega) \left[ \frac{r^2 \bar{V}^2}{\omega - E_f} - \frac{r^2 (V + \Delta V)^2}{\omega - E_f} \right] \\ &= -(1-c) \left( \frac{rV + S_{fc}}{\omega - E_f - S_{ff}} - \frac{rV}{\omega - E_f} \right) \\ & \quad - c \left[ \frac{rV + S_{fc}}{\omega - E_f - S_{ff}} - \frac{r(V + \Delta V)}{\omega - E_f} \right] \end{aligned} \quad (\text{A4})$$

from  $\mathbf{c}^T \mathcal{U} \mathbf{b} = 0$  and

$$\begin{aligned} & \left( \frac{rV + S_{fc}}{\omega - E_f - S_{ff}} - \frac{rV}{\omega - E_f} \right) F_{cc}(\omega) \left[ \frac{rV + S_{cf}}{\omega - E_f - S_{ff}} - \frac{r(V + \Delta V)}{\omega - E_f} \right] \\ &= \frac{1}{\omega - E_f} - \frac{1}{\omega - E_f - S_{ff}} \end{aligned} \quad (\text{A5})$$

from  $\mathbf{c}^T \mathcal{U} \mathbf{c} = 0$ . Equation (A2) can be easily reduced to the simplified CPA equation (18). Combining (A3) and (A4) with (A2), we obtain the relation (21). By substituting (17) into (13), (21) and (22) into (14) and (15), and (16) and (21) into (A5), equations (23)–(25) can be derived.

## References

- [1] Stewart G R 1984 *Rev. Mod. Phys.* **56** 755
- [2] Lee P A, Rice T M, Serene J W, Sham L J and Wilkins J W 1986 *Comment. Condens. Matter Phys.* **12** 99
- [3] Aeppli G, Yoshizawa H, Endoh Y, Bucher E, Hufnagl J, Onuki Y and Komatsubara T 1986 *Phys. Rev. Lett.* **57** 122
- [4] Uemura Y J et al 1989 *Phys. Rev. B* **39** 4726
- [5] Aeppli G, Bucher E, Broholm K, Kjems J K, Baumann J and Hufnagl J 1988 *Phys. Rev. Lett.* **60** 615
- [6] Gangopadhyay A K, Schilling J S, Schubert E, Gutmiedl P, Gross F and Andres K 1988 *Phys. Rev. B* **38** 2603
- [7] Germann A, Nigam A K, Dutzi J, Schröder A and Löhneysen H U 1988 *J. Physique Coll.* **49** C8 755
- [8] Lees M R and Coles B R 1988 *J. Magn. Magn. Mater.* **76–77** 173
- [9] Fraunberger G, Andraka B, Kim J S, Ahlheim U and Stewart G R 1989 *Phys. Rev. B* **40** 4735
- [10] Lees M R, Roy S B, Stewart G R and Coles B R 1990 *J. Phys.: Condens. Matter* **2** 4773
- [11] Zemirli S and Barbara B 1985 *Solid State Commun.* **56** 385
- [12] Xu W and Li Z Z 1988 *J. Phys. C: Solid State Phys.* **21** 4083
- [13] Li Z Z, Xu W, Chen C and Xiao M 1994 *Phys. Rev. B* **50** 11 332
- [14] de Visser A, Franse J J M, Lacerda A, Haen P and Flouquet J 1990 *Physica B* **163** 49
- [15] Brodale G E, Fisher R A, Phillips N E and Flouquet J 1986 *Phys. Rev. Lett.* **56** 390
- [16] Shisata A, Oomi G, Onuki Y and Komatsubara T 1986 *J. Phys. Soc. Japan* **55** 2086
- [17] Tešanović Z 1986 *Phys. Rev. B* **34** 5251

- [18] Rice T M and Ueda K 1986 *Phys. Rev. B* **34** 6420
- [19] Shi D, Xu W and Li Z Z 1988 *Solid State Commun.* **68** 171
- [20] Xu X, Li Z Z and Chen C 1995 *J. Phys.: Condens. Matter* **7** 2293
- [21] Chen C, Li Z Z and Xu W 1993 *J. Phys.: Condens. Matter* **5** 95
- [22] Chen C and Li Z Z 1994 *J. Phys.: Condens. Matter* **6** 2957
- [23] Tešanović Z and Valls O T 1986 *Phys. Rev. B* **34** 1918
- [24] Mills A and Lee P A 1987 *Phys. Rev. B* **35** 3394
- [25] Barnes S E 1976 *J. Phys. F: Met. Phys.* **6** 1375; 1977 *J. Phys. F: Met. Phys.* **7** 2631
- [26] Coleman P 1984 *Phys. Rev. B* **29** 3035
- [27] Yonezawa F 1982 *The Structure and Properties of Matter* ed T Matsubara (Berlin: Springer) ch 11
- [28] Xu W and Li Z Z 1990 *J. Phys.: Condens. Matter* **2** 109