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Theory for effects of pressure on heavy-fermion alloys

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The effects of pressure on heavy-fermion alloys are studied in the framework of the Yoshimori-Kasai model under the coherent potential approximation. A unified picture is presented for both electron-type heavy-fermion systems and hole-type heavy-fermion systems. The density of states of *f* electrons is calculated over the whole range of doping concentration under applied pressure. The Kondo temperature, the specific-heat coefficient, and the electrical resistivity are obtained, in agreement with the experiments qualitatively. The contrasting pressure-dependent effects for two types of heavy-fermion alloys are discussed to reveal the coherence in the system under pressure.

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I. INTRODUCTION

During the past two decades, considerable attention has been focused on heavy-fermion (HF) systems.[1–5] Generally speaking, HF systems are a class of intermetallic compounds which contain a periodic array of magnetic Kondo ions, involving rare earth $(4f)$ or actinide $(5f)$ elements. At higher temperatures than the Kondo temperature T_K, the localized magnetic moments behave essentially as independent impurities and each *f* electron becomes the scattering center in the Kondo effect. In this temperature region, the characters of the *f* electrons are similar to those in dilute alloys. At low temperatures, the coherent heavy fermion (or Fermi liquid) behaviors are observed, and the *f* electrons form a coherent Kondo lattice. The specific-heat coefficient γ is of the order of 10^2–10^3 larger than that of normal metals, and the density of states near the Fermi level, deduced from γ, is enhanced enormously. It is widely accepted that the large specific-heat coefficient is caused by the Kondo effect at each Kondo ion site.[1]

From the ensuing experimental and theoretical works, it is clear that HF materials, such as $\mathrm{CeAl_3}$,[6–9] $\mathrm{CeCu_6}$,[9–14] $\mathrm{UBe_{13}}$,[14–17] and $\mathrm{CeCu_2Si_2}$,[18,19] display many of the characteristics of a metallic Kondo lattice (KL), where a lattice of localized magnetic moments coexists with a conduction band.[20] Instead of a Kondo resonance (single-peak) structure in the impurity case, the density of states of *f* electrons (*f*-DOS) has a pseudogap (two-peak) structure near the Fermi level in the KL case, due to the periodic coherence between Kondo ions in the lattice. In order to get information on the development of coherence in HF systems, many experiments have been performed to study the alloying effects in doped HF systems, such as $\mathrm{Ce}_x\mathrm{La}_{1-x}\mathrm{Cu_2Si_2}$,[21–23] $\mathrm{Ce}_x\mathrm{La}_{1-x}\mathrm{Al_3}$,[24] $\mathrm{Ce}_x\mathrm{La}_{1-x}\mathrm{Be_{13}}$,[25] $\mathrm{Ce}_x\mathrm{La}_{1-x}\mathrm{Cu_6}$,[26–29] and so on. It is shown that, with an increase of the concentration of Kondo ions (Ce-like ions), an HF alloy system undergoes a crossover from the Kondo impurity state to the KL state. That is, doping Kondo ions present a consecutive approach to the coherent Kondo state efficiently. Meanwhile, the electrical resistivity ρ follows the quadratic law on temperature T in the KL case, which is one of the characteristic features of coherence, corresponding to the Fermi liquid behavior. Additionally, a shift of the peak in the specific-heat coefficient γ is observed to finite temperature with increasing of the concentration x,[23,24] while the Kondo temperature T_K is independent of x from experiments.[22,26,29] Theoretically, a dispersion term of the *f* electron band was introduced into the Anderson lattice model (ALM) by Yoshimori and Kasai to get a metallic KL system in the case of half-filling.[30] Under the coherent potential approximation (CPA), they calculate the electrical resistivity of HF alloys, and some excellent results are obtained, in agreement with experiments very well. Furthermore, Li and Qiu[31] extended the method of Yoshimori and Kasai, and tried to present a reasonable picture for heavy-fermion alloys by the application of the slave-boson mean-field approximation. They calculated the density of states, the thermoelectric power, the specific-heat coefficient, and the residual resistivity. The results themselves look meaningful and the obtained Kondo temperature T_K is indeed independent of the alloy concentration. While the slave-boson parameter has not been calculated over the whole range of the concentration $0 \leqslant x \leqslant 1$, their results seem artificial and more careful study is necessary even for the alloying effects of HF systems.

On the other hand, it is also possible to study systematically the development of the HF behaviors through the application of pressure. From the pressure-dependent measurements on $\mathrm{CeAl_3}$,[6–9] $\mathrm{CeCu_6}$,[9–14] $\mathrm{UBe_{13}}$,[14–16] $\mathrm{CeInCu_2}$,[32–36] $\mathrm{YbCu_2Si_2}$,[37,38] YbCuAl,[38,39] etc., it is clear that, for Ce-based and U-based HF systems, the specific-heat coefficient is depressed and the temperature $T_{\max}$, at which the electronic resistivity becomes the maximum, shifts to higher temperature under pressure. Furthermore, pressure tends to expand the temperature region of the quadratic law and to enhance the coherence of the system, while for Yb-based HF systems, just the opposite effects appear under pressure. More generally, pressure qualitatively acts as a *mirror* between Ce-based, U-based, and Yb-based compounds.[37,38] From experiments, pressure destabilizes the larger ion. In the case of *f*-electron systems, pressure will stabilize the f^{n-1} configuration relative to f^n.[16,40,41] For Ce-based compounds, the nonmagnetic $4f^0$ configuration would be favored rather than $4f^1$ under pressure,[14] while for Yb-based compounds, the magnetic $4f^{13}$ configuration would be favored under pressure rather than $4f^{14}$.[14,42] Moreover, pressure tends to induce a crossover from a localized *f*-electron states to an itinerant or coherent one for Ce-based compounds,[33,36] and the opposing effect is also expected for Yb-based compounds.[37,14] Although these important results stated above have been obtained from experiments for a long time, to the best of our knowledge, few works have been performed for the pressure effects on the HF systems theoretically. Among various possible approaches to study the pressure effects, the Kondo collapse (KC) is considered as a reasonable mechanism. It can be used to explain such fact that the hybridization V is very exponentially sensitive to pressure. But the KC theory also indicates that the volume decrease results in a large increase in the Kondo temperature.[20] It is true for the Ce-based[33–36] and U-based,[15,16] compounds, but not true for the Yb-based compounds where the volume decrease results in a decrease in the Kondo temperature.[37] So such a mechanism, the KC, is still controversial, and it seems not so efficient to think that the mirror effect between Ce-based, U-based, and Yb-based compounds can be explained within the framework of the KC. The essential of the problem is how pressure influences the development of coherence, in which the system displays typical HF features. Taking into account the valence fluctuation of f ions between the singlet and magnetic multiplet configurations, the pressure-dependent behaviors may arise from the cell-volume difference between f configurations. Pressure favors the f configuration with a smaller volume.[43,44] On this basis, we would like to develop a theory of pressure on HF alloys involving effects of doping and effects of pressure simultaneously. Following Li and Qiu,[31] the alloying effects of HF systems are studied within the Yoshimori-Kasai (YK) model by using the slave-boson mean-field approximation (SBMFA), but the main results are calcultated again over the whole range of the concentration $0\leqslant x\leqslant 1$ carefully in order to promote the credit of the method. The aim of the paper is to present a unified picture of pressure effects for both Ce-based, U-based, and Yb-based systems.

The rest of the paper is prepared as follows. In Sec. II, we formulate the disorder scattering within the mean-field approximation of YK model and introduce the volume variable to describe the pressure influence via the f valence fluctuation, originating from the hybridization between f electrons and conduction electrons (c electrons). Then the spectral function of the single-particle Green's function (GF) is obtained using the CPA method and a set of self-consistent equations is also addressed. Based on these, the f-DOS is performed numerically in Sec. III, while the specific-heat coefficient and the electrical resistivity are discussed in detail in Sec. IV, where we attempt to explain and compare the contrasting effects of pressure on Ce-based, U-based, and Yb-based systems in a unified theory. Finally, our results are summarized and discussed in Sec. V.

II. CPA DISORDER FORMALISM AND PRESSURE MODEL FOR HF ALLOYS

In the alloy systems such as $Ce_xLa_{1-x}Cu_2Si_2$, and $Ce_xLa_{1-x}Al_3$, there exist two kinds of rare earth atoms A and B, where A (Ce like) is a magnetic atom with f electrons and B (La like) a nonmagnetic atom without f electrons. The substitution of an A atom by a B atom introduces the disorder into the system and creates missing f electrons, referred to as Kondo holes. Following Li and Qiu,[31] the random variable at the lattice point l is defined by

$$\xi_l=\begin{cases}1 & \text{for } l\in A,\\ 0 & \text{for } l\in B,\end{cases} \tag{1}$$

and $\overline{\xi_l}=x$, the normalized concentration of A atoms. The YK model is the Anderson lattice model, with a small dispersion on f electron band,[30] and the disorder Hamiltonian can be written as

$$\begin{aligned}H=&\sum_{\mathbf{k}m}[\varepsilon_{\mathbf{k}}c^{\dagger}_{\mathbf{k}m}c_{\mathbf{k}m}+(\alpha\varepsilon_{\mathbf{k}}-E_0)f^{\dagger}_{\mathbf{k}m}f_{\mathbf{k}m}]\\&+\sum_{lm}(1-\xi_l)(E_L+E_0)f^{\dagger}_{lm}f_{lm}+V\sum_{lm}\xi_l(f^{\dagger}_{lm}c_{lm}\\&+c^{\dagger}_{lm}f_{lm})+\frac{1}{2}U\sum_{l,m\neq m'}\xi_l f^{\dagger}_{lm}f_{lm}f^{\dagger}_{lm'}f_{lm'},\end{aligned} \tag{2}$$

where $-E_0$ and E_L are the energy levels of f electrons on the A sites and B sites, respectively. $\varepsilon_{\mathbf{k}}$ is the energy of c electrons from Fermi level, which is assumed to be zero. U gives the on-site Coulomb repulsion between f electrons and V the c-f mixing parameter. The dispersion term $\alpha\varepsilon_{\mathbf{k}}$ is introduced into the YK model to get the metallic states even in the case of half-filling and the parameter α is proportional to V^2. Other notation in Eq. (2) is standard.

In the strong correlation limit $U\rightarrow\infty$, double occupation on A sites is forbidden and the Coleman's slave-boson (SB) operator b_l is introduced in the c-f mixing term.[45] Then the YK Hamiltonian (2) in SB formalism reads

$$\begin{aligned}H=&\sum_{\mathbf{k}m}[\varepsilon_{\mathbf{k}}c^{\dagger}_{\mathbf{k}m}c_{\mathbf{k}m}+(\alpha\varepsilon_{\mathbf{k}}-E_0)f^{\dagger}_{\mathbf{k}m}f_{\mathbf{k}m}]\\&+\sum_{lm}(1-\xi_l)(E_L+E_0)f^{\dagger}_{lm}f_{lm}+V\sum_{lm}\xi_l(b_l f^{\dagger}_{lm}c_{lm}\\&+c^{\dagger}_{lm}f_{lm}b^{\dagger}_l)+\sum_l\xi_l\lambda_l\left(\sum_m f^{\dagger}_{lm}f_{lm}+b^{\dagger}_l b_l-1\right),\end{aligned} \tag{3}$$

where a constraint

$$\sum_m f^{\dagger}_{lm}f_{lm}+b^{\dagger}_l b_l=1 \quad \text{for } l\in A \tag{4}$$

has been added with the Lagrange multiplier λ_l. Such a constraint prevents the double occupancy of f level on A sites due to the infinite U.

In order to consider the effects of pressure, let us introduce the total volume operator. In pure KL systems ($x=1$), such as $CeCu_6$, UBe_{13}, YbCuAl, etc., there is a lattice of rare earth or actinide ions which can exist in two valence states:[45,46] One of them is typically a singlet, $f^n(j=0)$ with zero j; the other a $2j+1(=N)$-fold-degenerate state, $f^{n+1}(j,+m)$ or $f^{n-1}(j,-m)$ with spin j. The weak hybridization between c electrons and the local f electrons causes the valence to fluctuate by the following changes in the f shell occupation:

$$f^{n+1}(j,+m) \rightleftharpoons f^{n}(j=0)+e^{-}(j,m) \quad \text{for Ce and U,} \tag{5}$$

$$f^{n-1}(j,-m) \rightleftharpoons f^{n}(j=0)+h^{+}(j,m) \quad \text{for Yb.} \tag{6}$$

According to the SB technique of Coleman[45]

$$|f^{n};j=0\rangle_l \equiv b_l^{\dagger}|0\rangle_l, \tag{7}$$

$$|f^{n\pm1};j,\pm m\rangle_l \equiv f_{lm}^{\dagger}|0\rangle_l. \tag{8}$$

Then at each site l, the valence fluctuation can be represented by a resonance between a zero-energy boson and a spin-j fermion in the subspace where $Q=n_b+n_f=1$. The fermion is an electron e^- for Ce and U, while a hole h^+ for Yb, respectively. In this paper, the numbers of channel $N(=2j+1)=2$ would be taken for simplicity, and two values $(\pm\frac{1}{2})$ are considered for m, written as σ from now on.

Taking into account the cell-volume difference $\Delta\Omega=\Omega_1-\Omega_0$ between two f configurations, we can write down the total volume operator as[43]

$$\Omega_t=\sum_l \Omega_l=\sum_l [b_l^{\dagger}b_l\Omega_0+(1-b_l^{\dagger}b_l)\Omega_1], \tag{9}$$

where Ω_0 and Ω_1 are the cell volume for the singlet f^n $(b_l^{\dagger}b_l=1)$ and the multiplet states $f^{n\pm1}$ $(b_l^{\dagger}b_l=0)$, respectively. Then, $\Delta\Omega$ is either positive for the cells with the electron-type (e-type) f ions (Ce and U) or negative for the cells with the hole-type (h-type) f ions (Yb). The more electrons occupy the f shell, the larger the ionic radius is.

In the case of alloy $(0\leqslant x\leqslant 1)$, we can express the total volume operator in terms of the random variable ξ_l as[44]

$$\Omega_t=\sum_l \{(1-\xi_l)\Omega_L+\xi_l[b_l^{\dagger}b_l\Omega_0+(1-b_l^{\dagger}b_l)\Omega_1]\}, \tag{10}$$

where Ω_L is the cell volume of a Kondo hole site (with La-like ions), and Ω_0 and Ω_1 are the cell volumes of an A atom in singlet f^n $(b_l^{\dagger}b_l=1)$ and multiplet $f^{n\pm1}(b_l^{\dagger}b_l=0)$ states, respectively.

In the SBMFA, the operator b_l and constraint (4) are replaced by their mean-field values with the ansatz $r=\langle b_l\rangle$ and $\lambda=\lambda_l$ for all A sites. Then the mean-field Hamiltonian is

$$\begin{aligned}H_{MF}=&\sum_{\mathbf{k}\sigma}[\varepsilon_{\mathbf{k}}c_{\mathbf{k}\sigma}^{\dagger}c_{\mathbf{k}\sigma}+(\alpha\varepsilon_{\mathbf{k}}+E_f)f_{\mathbf{k}\sigma}^{\dagger}f_{\mathbf{k}\sigma}]\\&+\sum_{l\sigma}(1-\xi_l)\varepsilon_L f_{l\sigma}^{\dagger}f_{l\sigma}+rV\sum_{l\sigma}\xi_l(f_{l\sigma}^{\dagger}c_{l\sigma}+c_{l\sigma}^{\dagger}f_{l\sigma})\\&+x\lambda N_s(r^2-1),\end{aligned} \tag{11}$$

where $E_f=\lambda-E_0$ and $\varepsilon_L=E_L-E_f$ are the renormalized f level of the magnetic (A) atoms and the Kondo holes (B atoms), respectively. Here we have used the relation $x=N_s^{-1}\Sigma_l\xi_l$, and N_s is the total number of sites in the system.

From Eq. (10), the averaged cell volume is

$$\bar{\Omega}_l=(1-x)\Omega_L+x[\Omega_0+(1-r^2)\Delta\Omega]. \tag{12}$$

Since pressure always decreases the averaged cell volume $\bar{\Omega}_l$, for the e-type HF systems (such as $\mathrm{CeCu_6}$ and $\mathrm{UBe_{13}}$) where $\Delta\Omega>0$, pressure will lead to the increasing of r^2, while for the h-type HF systems (such as YbCuAl), an opposite effect appears since $\Delta\Omega<0$.

Because a Kondo hole doping will lead to a very strong scattering, $E_L\to\infty$, so that $\varepsilon_L\to\infty$. We should solve the disorder slave-boson mean-field Hamiltonian (11) for arbitrary concentrations by means of a nonperturbative approach, the CPA.[47–49] Here, we would like to give the full steps to get the analytic solution of the coherent potential, instead of the procedure by Li and Qiu,[31] where such a solution is introduced directly.

To perform the CPA, we should introduce a translationally invariant but frequency-dependent coherent potential of the effective medium to replace the disorder scattering potential in Hamiltonian (11). The coherent potential for a c-f mixing model such as the YK model could be assumed as a 2×2 matrix[31,44,50]

$$S(\omega,x)=\begin{pmatrix}S_{cc} & S_{cf}\\ S_{fc} & S_{ff}\end{pmatrix}, \tag{13}$$

and the average site GF of the effective medium is obtained:

$$F(\omega)=\frac{1}{N_s}\sum_{\mathbf{k}}\bar{G}(\omega,\mathbf{k})=\begin{pmatrix}F_{cc}(\omega) & F_{cf}(\omega)\\ F_{fc}(\omega) & F_{ff}(\omega)\end{pmatrix}. \tag{14}$$

Then the effective medium Hamiltonian can be written in the matrix form

$$\begin{aligned}\bar{H}=&\sum_{\mathbf{k}\sigma}(c_{\mathbf{k}\sigma}^{\dagger}\quad f_{\mathbf{k}\sigma}^{\dagger})\begin{pmatrix}\varepsilon_{\mathbf{k}}+S_{cc} & S_{cf}\\ S_{fc} & (\alpha\varepsilon_{\mathbf{k}}+E_f)+S_{ff}\end{pmatrix}\begin{pmatrix}c_{\mathbf{k}\sigma}\\ f_{\mathbf{k}\sigma}\end{pmatrix}\\&+x\lambda N_s(r^2-1).\end{aligned} \tag{15}$$

From the difference between the disorder Hamiltonian (11) and the effective medium Hamiltonian (15),

$$H_{MF}-\bar{H}=\sum_l V_l, \tag{16}$$

the scattering potentials for atoms A and B are reached:

$$V_A=\begin{pmatrix}-S_{cc} & rV-S_{cf}\\ rV-S_{fc} & -S_{ff}\end{pmatrix},\quad V_B=\begin{pmatrix}-S_{cc} & -S_{cf}\\ -S_{fc} & \varepsilon_L-S_{ff}\end{pmatrix}. \tag{17}$$

According to Yonezawa,[49] the self-consistent condition in the single-site CPA is

$$xt_A+(1-x)t_B=0, \tag{18}$$

where t_A and t_B are the scattering t matrices for A and B atoms, respectively:

$$t_{A(B)}=V_{A(B)}[1-F(\omega)V_{A(B)}]^{-1}. \tag{19}$$

From Eqs. (17), (18), and (19), and taking $\varepsilon_L \to \infty$ to ensure no f electron occupation on Kondo holes, we can find an analytic solution of the coherent potential

$$S(\omega,x)=\begin{pmatrix} 0 & rV \\ rV & S_{ff} \end{pmatrix}, \tag{20}$$

where $S_{cc}=0$, $S_{cf}=S_{fc}=rV$, and only S_{ff} is to be determined. At the same time, the scattering t matrices can be simplified as

$$t_A=\frac{1}{1+S_{ff}F_{ff}}\begin{pmatrix} 0 & 0 \\ 0 & -S_{ff} \end{pmatrix}, \quad t_B=\frac{1}{F_{ff}}\begin{pmatrix} 0 & 0 \\ 0 & -1 \end{pmatrix}, \tag{21}$$

and the self-consistent CPA equation (18) can be written as

$$S_{ff}F_{ff}=x-1. \tag{22}$$

Now, the analytic solution of $S(\omega,x)$ and the self-consistent CPA equation are obtained after the detail derivation. These expressions are the same as those in the paper by Li and Qiu,[31] but the approach to them are not given there. Then, the average site GF's are expressed as

$$F_{cc}(\omega)=\frac{1}{N_s}\sum_{\mathbf{k}}\frac{\omega-\alpha\varepsilon_{\mathbf{k}}-E_f-S_{ff}}{(\omega-\varepsilon_{\mathbf{k}})(\omega-\alpha\varepsilon_{\mathbf{k}}-E_f-S_{ff})-(rV)^2}, \tag{23}$$

$$\begin{aligned} F_{cf}(\omega)&=F_{fc}(\omega) \\ &=\frac{1}{N_s}\sum_{\mathbf{k}}\frac{rV}{(\omega-\varepsilon_{\mathbf{k}})(\omega-\alpha\varepsilon_{\mathbf{k}}-E_f-S_{ff})-(rV)^2}, \end{aligned} \tag{24}$$

$$F_{ff}(\omega)=\frac{1}{N_s}\sum_{\mathbf{k}}\frac{\omega-\varepsilon_{\mathbf{k}}}{(\omega-\varepsilon_{\mathbf{k}})(\omega-\alpha\varepsilon_{\mathbf{k}}-E_f-S_{ff})-(rV)^2}, \tag{25}$$

which are also very different from those in the paper by Li and Qiu.[31]

The parameters of the SB, r and λ, can be determined by the extreme values of the grand canonical free enthalpy's variations (or, equivalently, by the Hellmann-Feynman theorem). The grand canonical free enthalpy of the HF alloy system under pressure p is

$$K=-\beta^{-1}\ln Z_{MF}, \tag{26}$$

where

$$Z_{MF}=\mathrm{Tr}\{\exp[-\beta(\overline{H}+p\Omega_t)]\}\equiv\mathrm{Tr}[\exp(-\beta H_{eff})]. \tag{27}$$

It is easy to write down the effective Hamiltonian of the SBMFA:

$$\begin{aligned} H_{eff}=\sum_{\mathbf{k}\sigma}&[\varepsilon_{\mathbf{k}}c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}+(\alpha\varepsilon_{\mathbf{k}}+E_f+S_{ff})f^\dagger_{\mathbf{k}\sigma}f_{\mathbf{k}\sigma} \\ &+rV(f^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}+c^\dagger_{\mathbf{k}\sigma}f_{\mathbf{k}\sigma})]+(1-x)N_s p\Omega_L \\ &+xN_s\{\lambda(r^2-1)+p[\Omega_0+(1-r^2)\Delta\Omega]\}. \end{aligned} \tag{28}$$

From the variation with respect to λ,

$$0=\frac{\delta K}{\delta\lambda}=\left\langle\frac{\partial H_{eff}}{\partial\lambda}\right\rangle_T=xN_s(r^2-1)+\sum_{\mathbf{k}\sigma}\langle f^\dagger_{\mathbf{k}\sigma}f_{\mathbf{k}\sigma}\rangle_T, \tag{29}$$

we get the equation including the parameter r,

$$\begin{aligned} x(1-r^2)&=\frac{1}{N_s}\sum_{\mathbf{k}\sigma}\langle f^\dagger_{\mathbf{k}\sigma}f_{\mathbf{k}\sigma}\rangle_T \\ &=-\frac{2}{\pi}\int_{-\infty}^{\infty}d\omega f(\omega)\mathrm{Im}F_{ff}(\omega+i0^+). \end{aligned} \tag{30}$$

And application of the same procedure to r,

$$\begin{aligned} 0=\frac{\delta K}{\delta r}=\left\langle\frac{\partial H_{eff}}{\partial r}\right\rangle_T&=V\sum_{\mathbf{k}\sigma}(\langle c^\dagger_{\mathbf{k}\sigma}f_{\mathbf{k}\sigma}\rangle_T+\langle f^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}\rangle_T) \\ &+2xN_s r(\lambda-p\Delta\Omega), \end{aligned} \tag{31}$$

implies another equation

$$\begin{aligned} xr(\lambda-p\Delta\Omega)&=-\frac{V}{N_s}\sum_{\mathbf{k}\sigma}\langle f^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}\rangle_T \\ &=\frac{2V}{\pi}\int_{-\infty}^{\infty}d\omega f(\omega)\mathrm{Im}F_{fc}(\omega+i0^+). \end{aligned} \tag{32}$$

Equations (22), (23), (24), (25), (30), and (32) constitute a set of self-consistent equations. These equations are not only fundamental to determine the coherent potential $S_{ff}(\omega,x)$ and the SB parameter r of the HF alloy systems, but also powerful for calculating the electronic DOS of both c electrons and f electrons with arbitrary alloy concentration under various applied pressures.

III. DENSITY OF STATES AND THE KONDO TEMPERATURE

The f-DOS per magnetic (A) site for each spin is defined by

$$N_f(\omega,p\Delta\Omega,x)=-\frac{1}{\pi x}\mathrm{Im}F_{ff}(\omega+i0^+), \tag{33}$$

where F_{ff} can be calculated self-consistently by numerical method. In the calculations, the unperturbed DOS of conduction electrons, $N_0(\omega)$, is assumed as[51]

$$N_0(\omega)=\frac{2}{\pi D}\sqrt{1-\left(\frac{\omega}{D}\right)^2}\Theta(D-|\omega|), \tag{34}$$

where $\Theta(x)$ is the step function and D the half-width of the unperturbed conduction band.

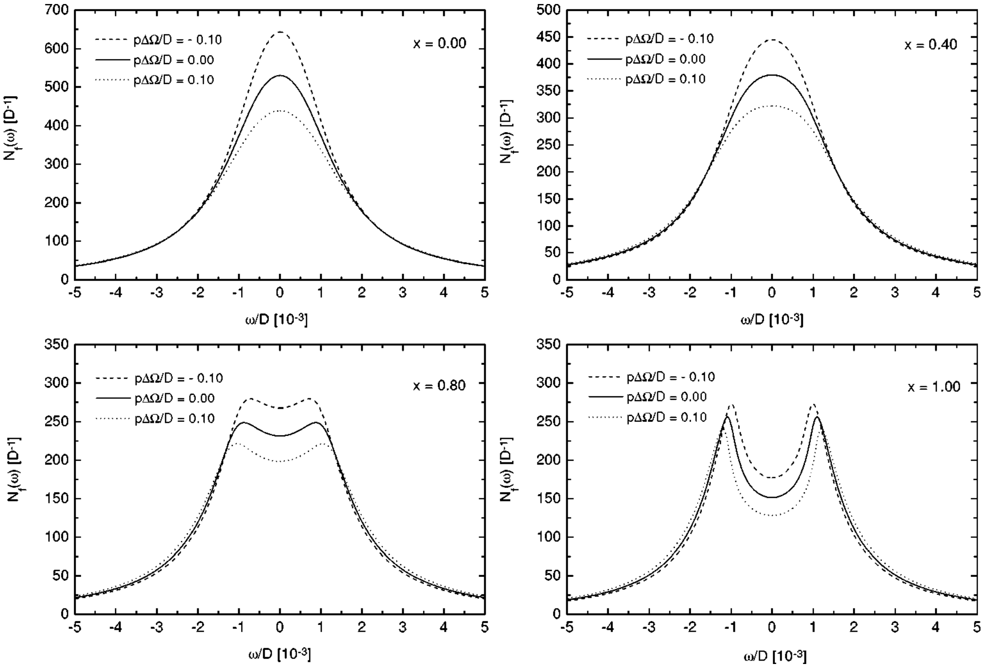

FIG. 1. Pressure effect on the *f*-DOS of HF alloys, for $x=0$, 0.4, 0.8, and 1.0. The parameters for the numerical calculation are $V^2=0.2D^2$, $E_0=1.2D$, and $\eta=1.05$.

In the case of a half-filled conduction band, $r^2 \ll 1$. From Eq. (4), $n_f \lesssim 1$ is obtained, corresponding to the Kondo limit associated with a large E_0.[46] Therefore, λ can be expected to be of order E_0,[52] and we can take $E_f=0$ and $\lambda=E_0$ as a reasonable approximation. The phenomenological parameter α in the dispersion term[53–55] can be written as[56]

$$\alpha=\eta^2\left(\frac{rV}{D}\right)^2, \tag{35}$$

where the parameter η is greater than 1 in order to get a metallic KL model without a real gap.[31]

The numerical results of the *f*-DOS are performed at various concentrations under applied pressure, shown in Fig. 1. It is clear that no real energy gap appears in the DOS of electrons for arbitrary concentration, and metallic behavior is obtained.

On the one hand, from Fig. 1, with the increasing of the concentration *x*, the *f*-DOS transforms from a Kondo impurity resonant state with a single-peak structure into a Kondo coherent state with a two-peak pseudogap structure. In the dilute region $(x \rightarrow 0)$ only a single peak appears, indicating the local impurity *f* states, the system behaves as a collection of independent Kondo singlet on each *A* site, and every *f* electron becomes the scattering center in the Kondo effect. When the concentration of *f* ions increases, the delocalization of the *f* electrons enhances due to the growing coherent scattering. After the concentration reaches a critical value, $x_c \lesssim 0.7$, for the parameters chosen for calculation here, the curve of the *f*-DOS near $\omega=0$ transforms into a concave shape from a convex one, showing the appearance of the coherent (two-peak) pseudogap state. In the high-concentration region $(x \rightarrow 1)$, the *f* electrons form a coherent lattice, a global Kondo singlet occurs, and the collection of independent Kondo singlets in dilute limit is replaced by a whole coherent Kondo lattice state here.

On the other hand, if pressure is applied, two different effects are reached for the *e*-type HF alloys $(\Delta\Omega>0)$ and the *h*-type HF alloys $(\Delta\Omega<0)$. For the *e*-type alloys, pressure increases the Kondo interaction and correlation between *f* ions (*A* sites),[14–16] and tends to enhance the itinerance of *f* electrons and the coherence of the system.[33,36] The width of the *f*-DOS near $\omega=0$ is broadened and the height is lowered under pressure, while for the *h*-type alloys, the opposing effect occurs. Pressure decreases the Kondo interaction and correlation between *f* ions, and tends to reduce the itinerance of *f* electrons and the coherence of the system.[14,37] The width of the *f*-DOS near $\omega=0$ is depressed and the height is lifted under pressure.

The effective mixing parameter $(rV)^2$ is also calculated out, shown in Fig. 2, over the whole range of alloy concentration $0 \leqslant x \leqslant 1$ under various pressures. On the one hand, with increasing concentration of *x*, $(rV)^2$ increases linearly and connects two well-known mean-field results, the Kondo impurity $(x \rightarrow 0)$ and the Kondo lattice $(x \rightarrow 1)$ naturally.[31] On the other hand, as shown in Fig. 2, the effect of pressure appears sensitively in the change of the effective mixing parameter. It is in agreement with experiments[14,37] qulitatively that pressure tends to promote an increase in hybridization and the mixing parameter but a decrease in localization for the *e*-type HF alloys $(\Delta\Omega>0)$, while conversely for the *h*-type HF alloys $(\Delta\Omega<0)$.

Furthermore, we would like to give some discussion on the pressure effects of the Kondo temperature. The Kondo temperature T_K is an energy scale, which is used to characterize the contribution to resistivity ρ with the temperature relation $\rho(T)=a-b\ln(T)$ due to the inelastic scattering of

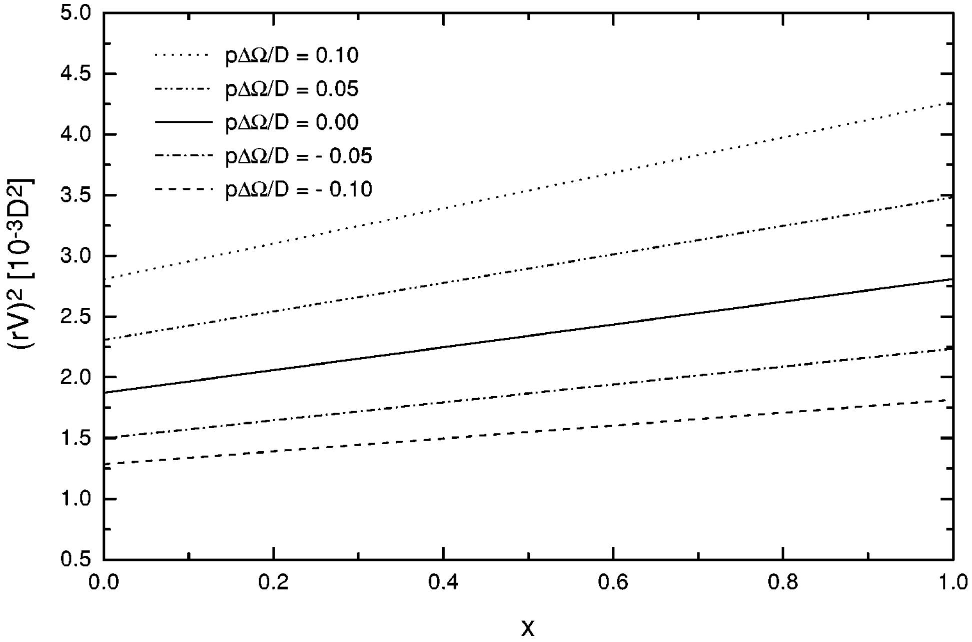

FIG. 2. Pressure effect on the effective mixing parameter $(rV)^2$ for the e-type $(\Delta\Omega>0)$ and the h-type $(\Delta\Omega<0)$ HF alloys over the whole range of x under various pressures.

conduction electrons from partially compensated local moments. With the decreasing of the temperature, a crossover occurs from the incoherent Kondo impurity state $(T>T_K)$ to the coherent KL state $(T<T_K)$. Theoretically, T_K can be determined in the limit $r\to 0$. From the self-consistent equations, it is directly obtained that

$$\frac{2V^2}{(\lambda-p\Delta\Omega)\pi}\int_{-\infty}^{\infty}d\omega\frac{1}{\exp\left(\frac{\omega}{k_BT_K}\right)+1}\frac{1}{N_s}\times\sum_{\mathbf{k}}\text{Im}\frac{1}{(\omega-\varepsilon_{\mathbf{k}}+i0^+)(\omega-E_f+i0^+)}=1, \tag{36}$$

and the expression for T_K reads

$$T_K=1.13\frac{D}{k_B}\exp\left(-\frac{E_0-p\Delta\Omega}{2N_0(0)V^2}\right). \tag{37}$$

This analytic expression for the Kondo temperature is given here explicitly as one of the important results of pressure effects. We would like to point out that such an expression does not appear in the paper by Li and Qiu,[31] where the case $p=0$ is considered and no effect of pressure is obtained.

From Eqs. (36) and (37), it is clear that the Kondo temperature T_K is independent of the concentration x, in agreement with the experiments.[22,26,29] On the other hand, as shown in Fig. 3, pressure increases the Kondo temperature T_K for the e-type HF systems $(\Delta\Omega>0)$, which is in agree-

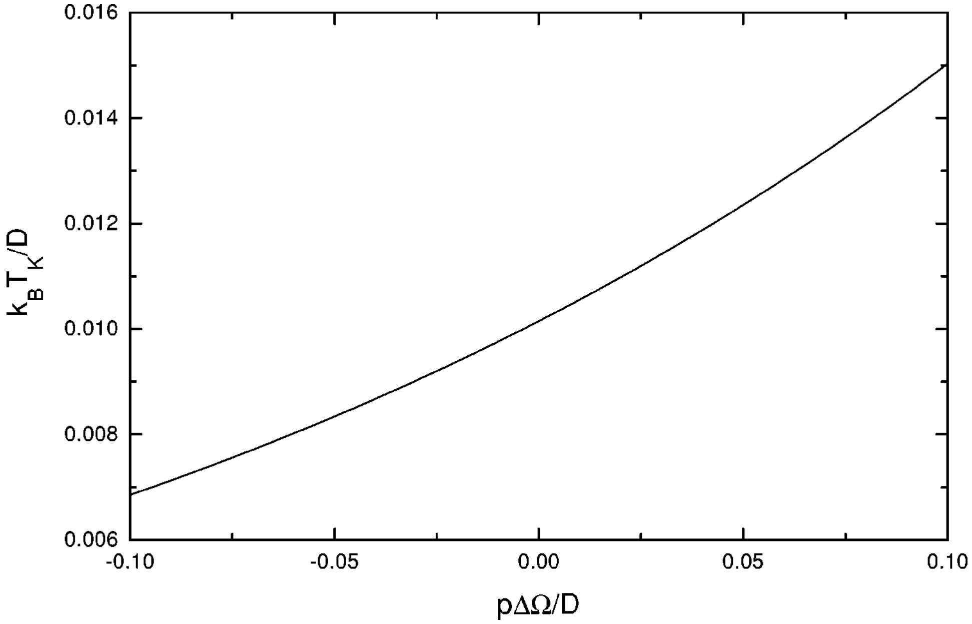

FIG. 3. Pressure effect on the Kondo temperature T_K for the e-type $(\Delta\Omega>0)$ and the h-type $(\Delta\Omega<0)$ HF alloys.

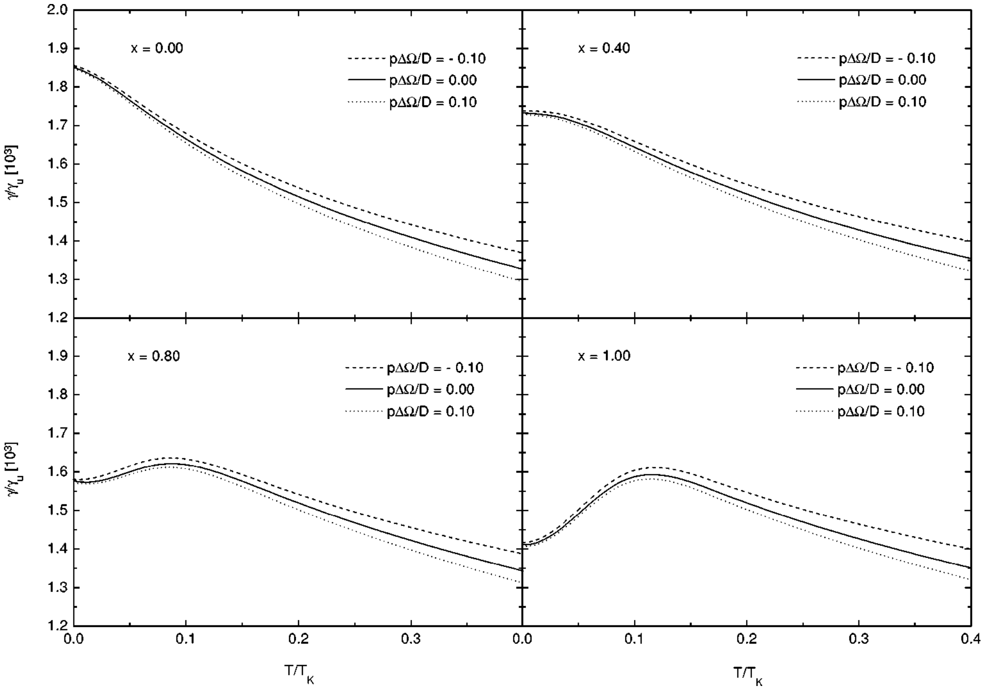

FIG. 4. Pressure effect on the specific-heat coefficient γ of HF alloys for $x=0$, 0.4, 0.8, and 1.0.

ment with the experiments on UBe_{13},[15,16] CeInCu_2,[33–36] and other *e*-type materials, while for the *h*-type HF systems $(\Delta\Omega<0)$, T_K decreases with the increment of pressure. Some experiments also indicate that the Kondo temperature T_K seems to decrease with pressure in the *h*-type compounds.[37]

According to the discussion about the *f*-DOS, the effective mixing parameter $(rV)^2$, and the Kondo temperature T_K, it is believed that pressure does act as a *mirror* between the *e*-type HF systems and the *h*-type HF systems unambiguously, in agreement with the experiments. Based on these results, we would calculate the specific-heat coefficient and the electrical resistivity to discuss the behaviors of HF system under pressure more intensively.

IV. COHERENCE EFFECTS UNDER PRESSURE

In the low-temperature region $T \ll T_K$, the main contribution of the specific heat arises from the thermal activation of *f* electrons near the Fermi level, and the specific-heat coefficient γ of HF alloys can be written in terms of the *f*-DOS as[31]

$$\gamma(T,p\Delta\Omega,x) = \frac{1}{2}k_B^2\beta^3\int_{-\infty}^{\infty} d\omega\,\omega^2 N_f(\omega,p\Delta\Omega,x)\,\mathrm{sech}^2\left(\frac{\beta\omega}{2}\right), \tag{38}$$

where $\beta=1/k_BT$. Then, from the *f*-DOS given above, the specific-heat coefficient γ can be obtained over the whole range of concentration x under various applied pressures (Fig. 4), the influence of pressure on T_K is also considered. It is shown that when $x<x_c$, the case of Kondo impurity, $\gamma(T)$ continues to increase monotonically as T decreases, indicating the incoherent state of the alloy system.[23] While in the KL case $(x>x_c)$, a maximum is found at a finite temperature well below T_K and a peak appears in each γ-T curve. With the increasing of concentration x, the peak shifts to higher temperature corresponding to the pseudogap structure. Generally, the maximum value of $\gamma(T)$, found at a finite temperature, is a characteristic feature of KL, which signals the transition to the coherent state and can be assigned experimentally to the effect of the periodicity of the system.[1,23,24]

On the other hand, as to the effect of pressure on the specific-heat coefficient γ, two opposing results are shown in Fig. 4. For the *e*-type HF alloys $(\Delta\Omega>0)$, pressure increases the correlation between *f* ions and promotes the itinerance of *f* electrons. The global Kondo singlet tends to be stabilized and the *f* multiplet states suppressed. Then, near the Fermi level, the *f*-DOS is lowered and the thermal activation decreases, leading to the decrement of γ under pressure. These results are in agreement with the measurements on the *e*-type HF systems CeAl_3,[8,9] CeCu_6,[13] UBe_{13},[17,9] and $\mathrm{CeCu}_2\mathrm{Si}_2$.[18] For the *h*-type HF alloys $(\Delta\Omega<0)$, pressure promotes the localization of *f* electrons, and tends to destabilize the global singlet state. The *f*-DOS near Fermi level is lifted and the thermal activation increases, leading to the increment of γ under pressure. These results are opposite to those of the *e*-type HF systems, as observed in YbCuAl,[39] etc.

From experiments, accompanying the decrease (increase) of γ for the *e*-type (*h*-type) HF systems is a rapid suppression (enhancement) of the T^2 coefficient A of the electrical resistivity ρ, an increase (decrease) of the temperature interval over which $\rho=\rho_0+AT^2$, and an increase (decrease) of the temperature T_{max} at which ρ has its maximum.[37,9,10,14] Study of the electrical resistivity ρ presents an effective ap-

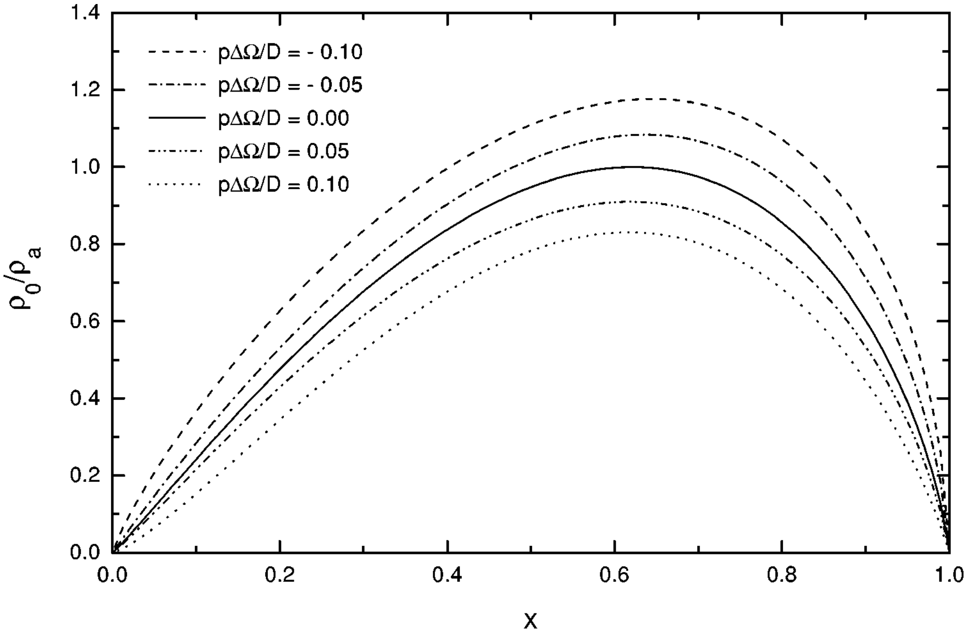

FIG. 5. Pressure effect on the residual resistivity ρ_0 over the whole range of the concentration x, where ρ_a is the maximum value of the curve $p=0$.

proach to reveal the effect of coherence in HF systems. According to the Kubo formula, the CPA expression of the electrical resistivity can be written as[48]

$$\sigma(T,p,x)=\frac{2e^2v_F^2}{3\pi\hbar^2\Omega}\int_{-\infty}^{\infty}d\omega\left(-\frac{\partial f}{\partial\omega}\right)\times\sum_{\mathbf{k}}\,[\mathrm{Im}\,\overline{G}_{cc}(\mathbf{k},p,\omega+i0^+)]^2, \tag{39}$$

where v_F is the Fermi velocity, Ω the volume of the system, and

$$\overline{G}_{cc}(\mathbf{k},p,\omega)=\frac{\omega-\alpha\varepsilon_{\mathbf{k}}-E_f-S_{ff}}{(\omega-\varepsilon_{\mathbf{k}})(\omega-\alpha\varepsilon_{\mathbf{k}}-E_f-S_{ff})-(rV)^2} \tag{40}$$

is the matrix element of the effective medium GF for conduction electrons.

At $T=0$, the residual resistivity $\rho_0(T=0,p,x)=1/\sigma(T=0,p,x)$ is calculated as shown in Fig. 5. It is found that ρ_0 has a maximum within $0\leqslant x\leqslant 1$ and approximately follows the Nordheim law $\rho_0\propto x(1-x)$.[22,25,26,29,30] On the other hand, for the e-type HF systems, ρ_0 decreases with increasing pressure, corresponding to the decrease in effective mass due to the enhancement of itinerance and coherence of the system under pressure,[33] which is in agreement with the ob-

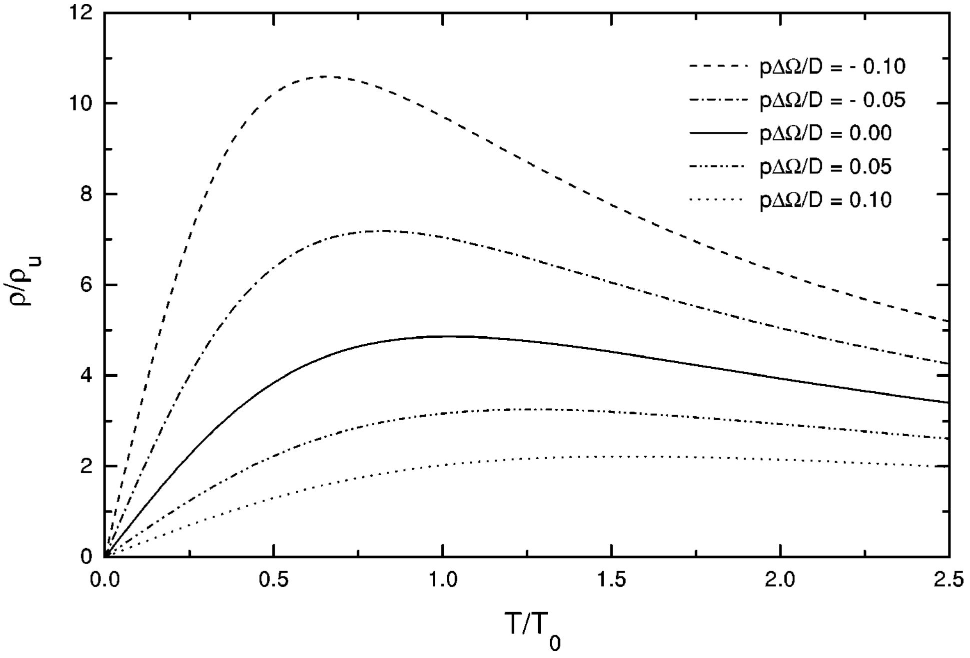

FIG. 6. Pressure effect on the electrical resistivity ρ of Kondo lattice $(x=1)$, where $\rho_u=3\pi\hbar^2D^2\Omega/2e^2v_F^2$ and T_0 is the $T_{\max}$ at $p=0$.

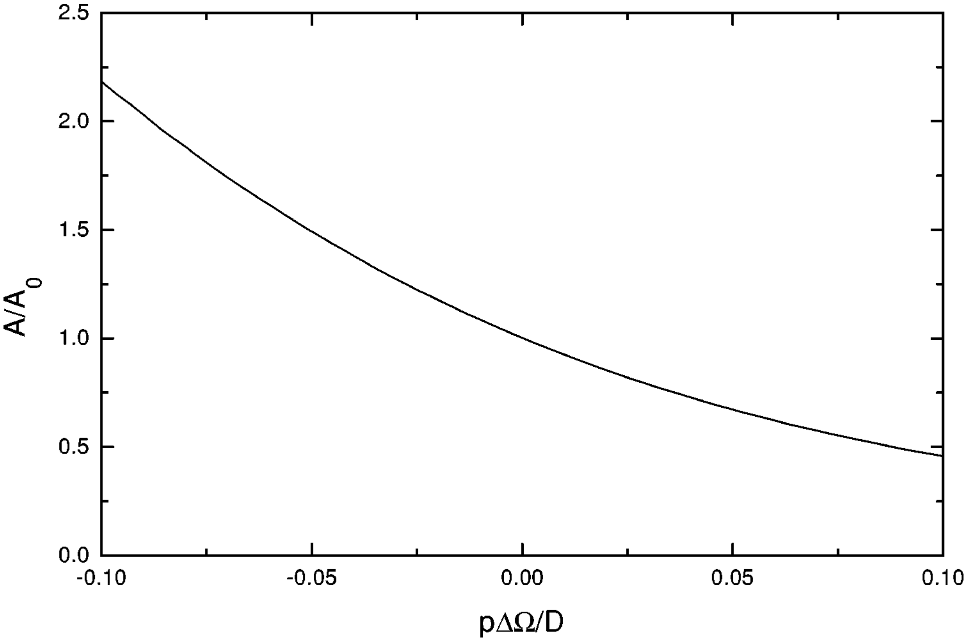

FIG. 7. Pressure effect on the coefficient A of the quadratic law of the resistivity in unit of A_0 for the Kondo model $(x=1)$, where A_0 is the value of the A at $p=0$.

servation in UBe_{13},[14–16] CeCu_6,[10,14] $\mathrm{CeCu}_2\mathrm{Si}_2$,[38] CeAl_3,[6,7] CeInCu_2,[33–36] etc, while for the *h*-type HF systems, ρ_0 increases with increasing pressure, corresponding to the increase in effective mass due to the enhancement of localization and incoherent state of the system under pressure,[14] as observed in YbAgCu_4,[37] $\mathrm{YbCu}_2\mathrm{Si}_2$,[37] etc. In the KL case $(x=1)$, the ρ-T curves are given in Fig. 6. The resistivity follows the quadratic law $\rho=\rho_0+AT^2$ (here, $\rho_0=0$ when $x=1$) at low temperature and has a maximum at $T_{\max}$. The coefficient A (Fig. 7) and the temperature $T_{\max}$ (Fig. 8) are strongly affected by the application of pressure. For the *e*-type HF systems, pressure increases the temperature $T_{\max}$ but decreases the coefficient A and expands the temperature region in which the quadratic law appears. Because the larger presence of the quadratic term in the temperature dependence of the resistivity accompanies the stronger coherence, these results indicate that pressure studies on the *e*-type HF systems provide a means of tuning the onset of Kondo coherence into the experimental temperature range without the introduction of disorder which accompanies doping.[15] For the *h*-type HF systems, pressure decreases $T_{\max}$ but increases the coefficient A and shrinks the temperature range for the quadratic law. Again, pressure acts as a mirror and leads to the contrasting effects on resistivity between the *e*-type HF systems, such as UBe_{13},[14–16] CeCu_6,[10,14] $\mathrm{CeCu}_2\mathrm{Si}_2$,[38]

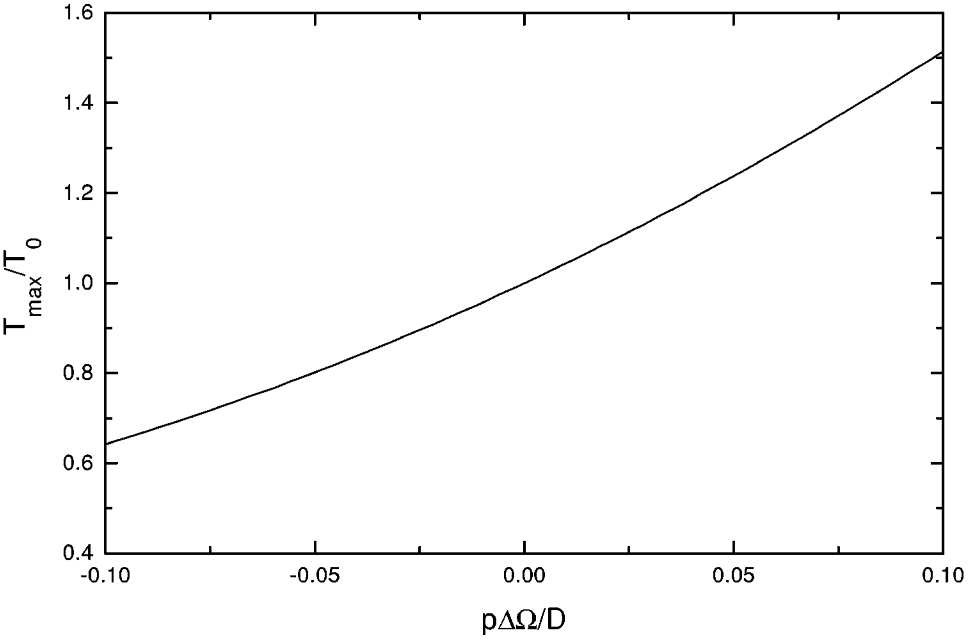

FIG. 8. Pressure effect on the temperature $T_{\max}$ at which ρ has its maximum for the Kondo model $(x=1)$, where T_0 is the $T_{\max}$ at $p=0$.

$CeAl_3$,[6,7] and $CeInCu_2$,[33–36] and the *h*-type HF systems, such as $YbAgCu_4$,[37] YbCuAl,[38] and $YbCu_2Si_2$.[37,38]

V. CONCLUSIONS

In this paper, the pressure effects on HF alloys are studied by the application of CPA in the framework of Yoshimori-Kasai model. Following Li and Qiu, the alloying effects of HF systems are studied by using the SBMFA. The density of states of f electrons, the Kondo temperature T_K, the specific-heat coefficient γ, and the electrical resistivity ρ are obtained in our CPA formalism for both the *e*-type HF alloys and the *h*-type HF alloys. It is found that with the increasing of the f ion concentration, as pointed out by Li and Qiu,[31] the system transforms from a Kondo impurity with single-peak structure into a coherent Kondo lattice with two-peak pseudogap structure. Accompanying this transformation, a peak appears in the specific-heat coefficient γ, and it shifts to higher temperature by increasing doping. On the other hand, pressure tends to enhance the itinerance and coherence of the system in the *e*-type HF alloys, while to support the localization and the incoherent state in the *h*-type HF alloys. The application of pressure increases the Kondo temperature and suppresses the specific-heat coefficient for the *e*-type HF systems. Accompanying these effects, pressure increases the temperature $T_{\max}$ and expands the temperature region for the quadratic law. Conversely, pressure decreases the Kondo temperature, enhances the specific-heat coefficient, and shrinks the temperature interval for the quadratic law in the *h*-type case. Our theoretical results on the HF systems can be looked on as a unified interpretation on the opposite pressure-dependent effects, observed in UBe_{13}, $CeCu_6$, $CeCu_2Si_2$, $CeAl_3$, and $CeInCu_2$ (the *e*-type HF systems) and $YbAgCu_4$, YbCuAl, and $YbCu_2Si_2$ (the *h*-type HF systems). Although, it is widely accepted that pressure acts qualitatively as a mirror between Ce-based, U-based, and Yb-based compounds,[37,38] further experiments are required to determine to what intensity and to what extent the *h*-type HF systems are mirror images of their *e*-type counterparts.

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