Pressure effects on the optical conductivity of Kondo insulators

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The effects of pressure on the optical conductivity of Kondo insulators are studied in the framework of the slave-boson mean-field theory under the coherent potential approximation. A unified picture is presented for both the hole-type Kondo insulators [H. Okamura *et al.*, Phys. Rev. B **58**, R7496 (1998)] and the electron-type Kondo insulators [B. Bucher *et al.*, Phys. Rev. Lett. **72**, 522 (1994)]. The density of states of f electrons under the applied pressure and its variation with the concentration of the impurity doping are calculated self-consistently. The Kondo temperature and the optical conductivity are obtained, in agreement with the experiments qualitatively. The two contrasting pressure-dependent effects for the hole-type Kondo insulators and the electron-type Kondo insulators are also given as predictions for further observations.

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I. INTRODUCTION

In recent years, many works have been focused on a class of strongly correlated materials, so-called Kondo insulators[1–14] such as $Ce_3Bi_4Pt_3$,[4,5] SmB_6,[6] and YbB_{12} [Ref. 7] etc. Generally speaking, Kondo insulators, or Kondo semiconductors are heavy-fermion compounds with insulating ground states, which contain rare earth $(4f)$ or actinide $(5f)$ elements, and exhibit very narrow energy gaps (E_g), typically 10–100 K, at low temperature. At higher temperature, especially above a characteristic temperature, Kondo temperature (T_K), Kondo insulators behave as local-moment metallic systems.[1,3] In various models based on the Anderson lattice Hamiltonian,[12–14] these distinguished properties of Kondo insulators are explained as results of the hybridization of f electrons and conduction electrons (c electrons) by strong-correlation effects.

In order to get information on the microscopic mechanism of the gap formation of Kondo insulators, infrared microwave measurements are used to address the crucial points.[15–19] The experiments of the infrared reflection and the optical conductivity on $Ce_3Bi_4Pt_3$,[19] SmB_6 [Refs. 15–17] and YbB_{12} [Ref. 18] present the picture of low-energy excitations and the main feature of the gap formation of Kondo insulators. At high temperature, the spectrum is still metallic, showing the temperature-dependent hybridization gap E_g diminished with increasing temperature.[18,19] While at low temperature, a significant amount of spectral weight (integrated conductivity) is strongly depleted from the low-frequency region. The spectrum is typical of an insulator (semiconductor) with an energy gap.[18] The extrinsic effects, including defects and impurities, also become dominant at low-temperature region,[19] and the gap formation would be influenced by them.

The characteristic behaviors of the gap formation and the optical conductivity of Ce-based Kondo insulator $Ce_3Bi_4Pt_3$ [Ref. 19] are very similar to those of Yb-based Kondo insulator YbB_{12}.[18] Without pressure, these behaviors, shared by the two representative Kondo insulators, are likely to be universal optical features of Kondo insulators. On the other hand, from the pressure-dependent measurements on $Ce_3Bi_4Pt_3$,[10] SmB_6,[9] and YbB_{12},[11] pressure appears to suppress the gaps of Sm-based and Yb-based Kondo insulators while just the opposite effect for Ce-based Kondo insulators. So the optical behaviors of these two kinds of Kondo insulators will be different under pressure. Although it is a very important and interesting problem, to the best of our knowledge, very few works have been performed for the pressure effects on the optical conductivity of Kondo insulators both in theories and in experiments. Theoretically, the central question of pressure effects on Kondo insulators is how pressure modifies the many-body effects that determine the development of the gap.[20,21] The pressure-dependent behavior may arise from the cell-volume difference between f configurations due to the valence fluctuation character of the f ions and their valence variations with pressure. Pressure favors the f configurations with smaller volume. On this basis, we develop a theory of pressure effects on the optical conductivity of Kondo insulators, using the slave-boson mean-field approximation (SBMFA) for the Anderson lattice model (ALM). Especially, the effect of impurity is considered as well as the volume effect, to establish the theory.

The rest of this paper is organized as follows. In Sec. II, we formulate the impurity scattering within the mean-field approximation of ALM and introduce the volume variable to describe the pressure influence via the f valence fluctuation, originating from the hybridization between f electrons and c electrons. Then the spectral function of single-particle Green's function (GF) is obtained using the coherent-potential approximation (CPA) method. In Sec. III, the self-consistent calculations on f electron's density of states (f-DOS) and the optical conductivities are performed numerically. We attempt to explain and compare two different pressure effects on $Ce_3Bi_4Pt_3$, SmB_6, and YbB_{12}. Finally, our results are summarized and discussed in Sec. IV.

II. IMPURITY MODEL AND CPA FORMALISM

The impurity effect of Kondo insulators discussed in this paper can be looked as disorder doping on the conduction band.[22] As an appropriate starting point for discussing doped Kondo insulators, we introduce a random scattering potential for the conduction electrons into the nondegenerate Anderson lattice model with a half-filled conduction band.[21,23] The

random variable in the lattice site l is defined by

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

where $A(B)$ is the lattice cell with (without) a scattering potential. Note that the random average $\overline{\xi_l^2}=\overline{\xi_l}=x$, where x is the normalized concentration of A (impurity doping) atoms.

The Hamiltonian of ALM is given by

$$H=\sum_{\mathbf{k}\sigma}\left[\varepsilon_{\mathbf{k}}c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}+E_0 f^{\dagger}_{\mathbf{k}\sigma}f_{\mathbf{k}\sigma}\right]+V\sum_{l\sigma}\left(c^{\dagger}_{l\sigma}f_{l\sigma}+f^{\dagger}_{l\sigma}c_{l\sigma}\right)+\frac{1}{2}U\sum_{l\sigma}f^{\dagger}_{l\sigma}f_{l\sigma}f^{\dagger}_{l\bar{\sigma}}f_{l\bar{\sigma}}, \tag{2}$$

where $c_{\mathbf{k}\sigma}$ ($c_{l\sigma}$) and $f_{\mathbf{k}\sigma}$ ($f_{l\sigma}$) are operators in Bloch (Wannier) representation for the conduction (c) electrons and localized f electrons, respectively. $\varepsilon_{\mathbf{k}}$ is the band energy of c electrons from the Fermi level and E_0 the energy of f electrons on B sites. V represents the c-f mixing parameter, while U the on-site Coulomb repulsion between two electrons with the opposite spin. σ gives the spin index.

If we introduce the scattering potential W for c electrons into the model,[22] the Hamiltonian becomes

$$H=\sum_{\mathbf{k}\sigma}\left[\varepsilon_{\mathbf{k}}c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}+E_0 f^{\dagger}_{\mathbf{k}\sigma}f_{\mathbf{k}\sigma}\right]+\sum_{l\sigma}\xi_l W c^{\dagger}_{l\sigma}c_{l\sigma}+V\sum_{l\sigma}\left(c^{\dagger}_{l\sigma}f_{l\sigma}+f^{\dagger}_{l\sigma}c_{l\sigma}\right)+\frac{1}{2}U\sum_{l\sigma}f^{\dagger}_{l\sigma}f_{l\sigma}f^{\dagger}_{l\bar{\sigma}}f_{l\bar{\sigma}}. \tag{3}$$

In the strong-correlation limit $U\to\infty$, double occupation on B sites is strictly forbidden. The Coleman's[24] slave-boson operator b_l is introduced in the c-f mixing term instead of Coulomb repulsion part in Eq. (3). So the Anderson lattice Hamiltonian can be written in the slave-boson formalism as

$$H=\sum_{\mathbf{k}\sigma}\left[\varepsilon_{\mathbf{k}}c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}+E_0 f^{\dagger}_{\mathbf{k}\sigma}f_{\mathbf{k}\sigma}\right]+\sum_{l\sigma}\xi_l W c^{\dagger}_{l\sigma}c_{l\sigma}+V\sum_{l\sigma}\left(b_l f^{\dagger}_{l\sigma}c_{l\sigma}+c^{\dagger}_{l\sigma}f_{l\sigma}b^{\dagger}_l\right)+\sum_l\lambda_l\left(\sum_{\sigma}f^{\dagger}_{l\sigma}f_{l\sigma}+b^{\dagger}_l b_l-1\right), \tag{4}$$

where a constraint due to infinite U

$$\sum_{\sigma}f^{\dagger}_{l\sigma}f_{l\sigma}+b^{\dagger}_l b_l=1 \quad \text{for } l\in B, \tag{5}$$

is added with the Lagrange multiplier λ_l. This constraint prevent the double occupancy of f level on the B sites.

In order to consider the effects of pressure, let us introduce the total volume operator. In pure Kondo insulators, the most typical valence-fluctuation ions Ce, Sm, and Yb can exist in two valence states:[25] One is a singlet, $f^n(j=0)$ with zero j; the others are the magnetic multiplet states $f^{n-1}(j,-m)$ and $f^{n+1}(j,+m)$ with nonzero j. The weak hybridization of conduction electrons with the local f electrons causes the valence to fluctuate by the following changes in the f-shell occupation:

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

$$f^{n+1}(j,+m)\rightleftharpoons f^n(j=0)+e^-(j,m) \quad \text{for Ce.} \tag{7}$$

In terms of Coleman's slave-boson technique,[24]

$$b^{\dagger}_l|0\rangle_l=|f^n{:}j=0\rangle_l, \tag{8}$$

$$f^{\dagger}|0\rangle_l=|f^{n\pm1}{:}j,\pm m\rangle_l, \tag{9}$$

where the singlet state of f ions for a site l is represented by a slave-boson field b_l and the magnetic multiplet states f^{n-1} and f^{n+1} by a fermion. The fermion is a hole h^+ for Sm, Yb and an electron e^- for Ce, respectively. Considering the cell-volume difference $\Delta\Omega=\Omega_1-\Omega_0$ between two f configurations, we can write down the total volume operator as[20]

$$\Omega_t=\sum_l\Omega_l=\sum_l\left[b^{\dagger}_l b_l\Omega_0+(1-b^{\dagger}_l b_l)\Omega_1\right], \tag{10}$$

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

In the case of impurity, we can express the total volume operator of doped Kondo insulators system in terms of random variable ξ_l as[21]

$$\Omega_t=\sum_l\left\{\xi_l\Omega_L+(1-\xi_l)\left[b^{\dagger}_l b_l\Omega_0+(1-b^{\dagger}_l b_l)\Omega_1\right]\right\}, \tag{11}$$

where Ω_L is the cell volume of an impurity site (A site), Ω_0 and Ω_1 are the cell volumes of a B site in singlet $f^n(b^{\dagger}_l b_l=1)$ and multiplet $f^{n\pm1}(b^{\dagger}_l b_l=0)$ states, respectively.

In the SBMFA, the operator b_l and constraint (5) are replaced by their mean-field values with the ansatz: $r=\langle b_l\rangle$ and $\lambda_l=\lambda$ for all B sites. Then the mean-field Hamiltonian is

$$H=\sum_{\mathbf{k}\sigma}\left[\varepsilon_{\mathbf{k}}c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}+E_f f^{\dagger}_{\mathbf{k}\sigma}f_{\mathbf{k}\sigma}\right]+\sum_{l\sigma}\xi_l W c^{\dagger}_{l\sigma}c_{l\sigma}+rV\sum_{l\sigma}\left(f^{\dagger}_{l\sigma}c_{l\sigma}+c^{\dagger}_{l\sigma}f_{l\sigma}\right)+N_s\lambda(r^2-1), \tag{12}$$

where $E_f=E_0+\lambda$ is the renormalized f level of B atoms. We have to solve the disorder slave-boson mean-field Hamiltonian (12) for arbitrary concentrations of the impurity by means of a nonperturbative approach, the CPA. Here we use the relation $x=N_s^{-1}\Sigma_l\xi_l$, and N_s is the number of sites in the system.

The idea of CPA is to replace the disorder scattering potential by a translational invariant but frequency-dependent coherent potential of the effective medium.[26,27] The coherent

potential for a c-f mixing model such as ALM should be assumed as a 2×2 matrix[21,23]

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

The effective medium Hamiltonian can be written in the matrix form

$$\overline{H}=\sum_{\mathbf{k}\sigma}\ (c^{\dagger}_{\mathbf{k}\sigma}f^{\dagger}_{\mathbf{k}\sigma})\begin{pmatrix} \varepsilon_{\mathbf{k}}+S_{cc} & S_{cf} \\ S_{fc} & E_f+S_{ff} \end{pmatrix}\begin{pmatrix} c_{\mathbf{k}\sigma} \\ f_{\mathbf{k}\sigma} \end{pmatrix}+N_s\lambda(r^2-1). \tag{14}$$

In Bloch representation, the matrix of the medium GF is determined by $(\omega-\overline{H})^{-1}$ in the space of basis vector $(c_{\mathbf{k}\sigma},f_{\mathbf{k}\sigma})$ and reads

$$\overline{G}(\omega,\mathbf{k})=\frac{1}{B_{\mathbf{k}}}\begin{pmatrix} \omega-E_f-S_{ff} & S_{cf} \\ S_{fc} & \omega-\varepsilon_{\mathbf{k}}-S_{cc} \end{pmatrix}, \tag{15}$$

with

$$B_{\mathbf{k}}=(\omega-\varepsilon_{\mathbf{k}}-S_{cc})(\omega-E_f-S_{ff})-S_{cf}S_{fc}\,. \tag{16}$$

From Eq. (15), we obtain the average site GF of the effective medium

$$F(\omega)=\frac{1}{N_s}\sum_{\mathbf{k}}\ \overline{G}(\omega,\mathbf{k})=\begin{pmatrix} F_{cc}(\omega) & F_{cf}(\omega) \\ F_{fc}(\omega) & F_{ff}(\omega) \end{pmatrix}. \tag{17}$$

The only remaining thing is to determine the coherent potential $S(\omega,\mathbf{k})$, which can be obtained by solving the self-consistent equations of the CPA. In the single-site CPA, the potential $S(\omega,\mathbf{k})$ has to be determined in such a way, that on an average, the scattering t matrix for the difference between potentials of the disorder system and the effective medium vanishes on each site. According to Yonezawa,[27] this requirement is equivalent to a self-consistent equation in single-site CPA

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

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

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

with scattering potential of A and B atoms between the effective medium and our disordered system

$$V_A=\begin{pmatrix} W-S_{cc} & rV-S_{cf} \\ rV-S_{fc} & -S_{ff} \end{pmatrix}, \tag{20}$$

and

$$V_B=\begin{pmatrix} -S_{cc} & rV-S_{cf} \\ rV-S_{fc} & -S_{ff} \end{pmatrix}. \tag{21}$$

Substituting Eqs. (20) and (21) into Eq. (18), we can find a analytic solution of the coherent potential

$$S(\omega,x)=\begin{pmatrix} S_{cc} & rV \\ rV & 0 \end{pmatrix}, \tag{22}$$

where $S_{ff}=0$, $S_{cf}=S_{fc}=rV$ and only the matrix element S_{cc} is unknown. At the same time, the self-consistent CPA equation (18) can be written as

$$F_{cc}S_{cc}^2-WF_{cc}S_{cc}+S_{cc}-xW=0. \tag{23}$$

Then, the average site GFs are expressed as

$$F_{cc}(\omega)=\frac{1}{N_s}\sum_{\mathbf{k}}\frac{\omega-E_f}{(\omega-\varepsilon_{\mathbf{k}}-S_{cc})(\omega-E_f)-(rV)^2}, \tag{24}$$

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

$$F_{ff}(\omega)=\frac{1}{N_s}\sum_{\mathbf{k}}\frac{\omega-\varepsilon_{\mathbf{k}}-S_{cc}}{(\omega-\varepsilon_{\mathbf{k}}-S_{cc})(\omega-E_f)-(rV)^2}. \tag{26}$$

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

$$K=-\beta^{-1}\ln Z_{MF}\,, \tag{27}$$

where

$$\begin{aligned} Z_{MF}&=\mathrm{Tr}\{\exp[-\beta(\overline{H}+p\Omega_t-\mu N_t)]\} \\ &\equiv\mathrm{Tr}\{\exp[-\beta(H_{eff}-\mu N_t)]\}. \end{aligned} \tag{28}$$

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

$$\begin{aligned} H_{eff}=\sum_{\mathbf{k}\sigma}\ &[(\varepsilon_{\mathbf{k}}+S_{cc})c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}+E_f f^{\dagger}_{\mathbf{k}\sigma}f_{\mathbf{k}\sigma} \\ &+rV(f^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}+c^{\dagger}_{\mathbf{k}\sigma}f_{\mathbf{k}\sigma})]+xN_sp\Omega_L+N_s\lambda(r^2-1) \\ &+(1-x)N_sp[\Omega_0+(1-r^2)\Delta\Omega]. \end{aligned} \tag{29}$$

From the variation with respect to λ,

$$0=\frac{\delta K}{\delta\lambda}=\left\langle\frac{\partial H_{eff}}{\partial\lambda}\right\rangle_T=N_s(r^2-1)+\sum_{\mathbf{k}\sigma}\ \langle f^{\dagger}_{\mathbf{k}\sigma}f_{\mathbf{k}\sigma}\rangle_T, \tag{30}$$

we get the equation including parameter r,

$$\begin{aligned} 1-r^2&=\frac{1}{N_s}\sum_{\mathbf{k}\sigma}\ \langle f^{\dagger}_{\mathbf{k}\sigma}f_{\mathbf{k}\sigma}\rangle_T \\ &=-\frac{2}{\pi}\int_{-\infty}^{\infty}d\omega f(\omega-\mu)\mathrm{Im}\,F_{ff}(\omega+i0^+). \end{aligned} \tag{31}$$

And the same procedure to r,

$$0=\frac{\delta K}{\delta r}=\left\langle\frac{\partial H_{eff}}{\partial r}\right\rangle_T=V\sum_{\mathbf{k}\sigma}(\langle c^\dagger_{\mathbf{k}\sigma}f_{\mathbf{k}\sigma}\rangle_T+\langle f^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}\rangle_T)+2N_s r[\lambda-(1-x)p\Delta\Omega], \tag{32}$$

implies another equation,

$$[\lambda-(1-x)p\Delta\Omega]r=-\frac{V}{2N_s}\sum_{\mathbf{k}\sigma}(\langle c^\dagger_{\mathbf{k}\sigma}f_{\mathbf{k}\sigma}\rangle_T+\langle f^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}\rangle_T)=\frac{2V}{\pi}\int_{-\infty}^{\infty}d\omega f(\omega-\mu)\mathrm{Im}F_{fc}(\omega+i0^+), \tag{33}$$

where we have used $F_{fc}(\omega)=F_{cf}(\omega)$, and $f(\omega)$ is the Fermi distribution function. The chemical potential μ can be obtained from the conservation of the total number of the particles

$$N_t=-\frac{\partial K}{\partial\mu}=(2-x)N_s, \tag{34}$$

where we have assumed that there is only one conduction electron per site for the disordered Kondo system. Equation (34) can be rewritten as

$$(2-x)=-\frac{2}{\pi}\int_{-\infty}^{\infty}d\omega f(\omega-\mu)\mathrm{Im}[F_{cc}(\omega+i0^+)+F_{ff}(\omega+i0^+)]. \tag{35}$$

Within SBMFA, the averaged cell volume is[21]

$$\overline{\Omega}_l=x\Omega_L+(1-x)[\Omega_0+(1-r^2)\Delta\Omega], \tag{36}$$

where

$$\Delta\Omega\equiv\Omega_1-\Omega_0. \tag{37}$$

Since the pressure always decreases the averaged cell volume $\overline{\Omega}_l$, for the electron-type Kondo insulators, such as $Ce_3Bi_4Pt_3$, $\Delta\Omega>0$, pressure will lead to the increasing of r^2. For the hole-type Kondo insulators, such as SmB_6 and YbB_{12}, an opposite effect exists since $\Delta\Omega<0$.

Eqs. (23)–(26), (31), (33), and (35) constitute a set of self-consistent equations, which can be used to determine the coherent potential $S_{cc}(\omega,x)$ and the electronic DOS of Kondo insulators with arbitrary impurity concentrations under various pressures.

III. THEORETICAL ANALYSIS AND DISCUSSION

The *f*-DOS of Kondo insulators under pressure is defined by the imaginary part of the effective-medium GF, $F_{ff}(\omega)$,

$$N_f(\omega,p\Delta\Omega,x)=-\frac{1}{\pi(1-x)}\mathrm{Im}F_{ff}(\omega+i0^+), \tag{38}$$

where $F_{ff}(\omega)$ can be calculated self-consistently from Eqs. (23), (26), (31), and (33) by numerical method. In the calculations, the unperturbed DOS of conduction electrons $N_0(\omega)$ is assumed as

$$N_0(\omega)=(1/2D)\Theta(D-|\omega|), \tag{39}$$

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

The numerical results of *f*-DOS and the Kondo temperature T_K are shown in Fig. 1 and Fig. 2, respectively. Pressure enhances Kondo interaction, hybridization gap, and T_K for the electron-type Kondo insulators ($\Delta\Omega>0$) and, on the contrary, suppresses them for the hole-type Kondo insulators ($\Delta\Omega<0$). On the other hand, it is also clear that an impurity band emerges within the gap near the edge of the lower band, and the band is broadened with increasing of the concentration x. It is very different from the case of doping Kondo holes into Kondo insulators,[23] where the impurity band emerges near the Fermi level. In our case here, the Kondo temperature T_K is dependent not only on the pressure but also on the impurity concentration. From Fig. 2, T_K increases with increasing concentration x.[28] This is another behavior apart from Kondo insulators by doping Kondo holes, where the Kondo temperature is independent of x according to the experiments.[29,30]

Based on the calculation of the optical conductivity of Kondo insulators, we will give some theoretical explanation on the experimental data for $Ce_3Bi_4Pt_3$,[19] SmB_6,[15–17] and YbB_{12}.[18] Although, to the best of our knowledge, there are no experimental results about the pressure effect on it, we would like to make some theoretical predictions here.

According to the Kubo formula,[31] (the real part of) the optical conductivity for an isotropic system is determined by the current-correlation function

$$\sigma_r(\omega,T)=\mathrm{Re}\,\sigma(\omega,T)=-\mathrm{Im}\frac{1}{\omega}\overline{\langle\langle j_z|j_z\rangle\rangle}_\omega, \tag{40}$$

where

$$j_z=e\sum_{\mathbf{k}\sigma}v_{\mathbf{k}z}c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}, \tag{41}$$

is the component of the current operator along an arbitrary direction z, and $\hbar\mathbf{v}_\mathbf{k}=\partial\varepsilon_\mathbf{k}/\partial\mathbf{k}$, the velocity of the conduction electron with wave vector $\mathbf{k}$ and energy $\varepsilon_\mathbf{k}$.[32] The bar in Eq. (40) means an average over the randomness due to the impurity doping. Only the contribution of conduction electrons to the current is taken into account. Then after some simple derivation, the optical conductivity of our system reads[33]

$$\sigma(\omega,p,T)=\frac{2e^2v_F^2}{3\pi\hbar^2}\int_{-\infty}^{\infty}d\nu\sum_{\mathbf{k}}[\mathrm{Im}\,\overline{G}_{cc}(\mathbf{k},p,\nu+i0^+)\times\mathrm{Im}\,\overline{G}_{cc}(\mathbf{k},p,\omega+\nu+i0^+)]\frac{[f(\nu)-f(\omega+\nu)]}{\omega}, \tag{42}$$

where σ_r is written as σ for simplicity and $\mathbf{v}_\mathbf{k}$ approximated by the Fermi velocity v_F due to the isotropic system.[32] In the framework of CPA, we have used the effective-medium GF $\overline{G}_{cc}(\mathbf{k})$ to express the disorder GF $\overline{\langle\langle c_{\mathbf{k}\sigma}|c^\dagger_{\mathbf{k}\sigma}\rangle\rangle}_\omega$.

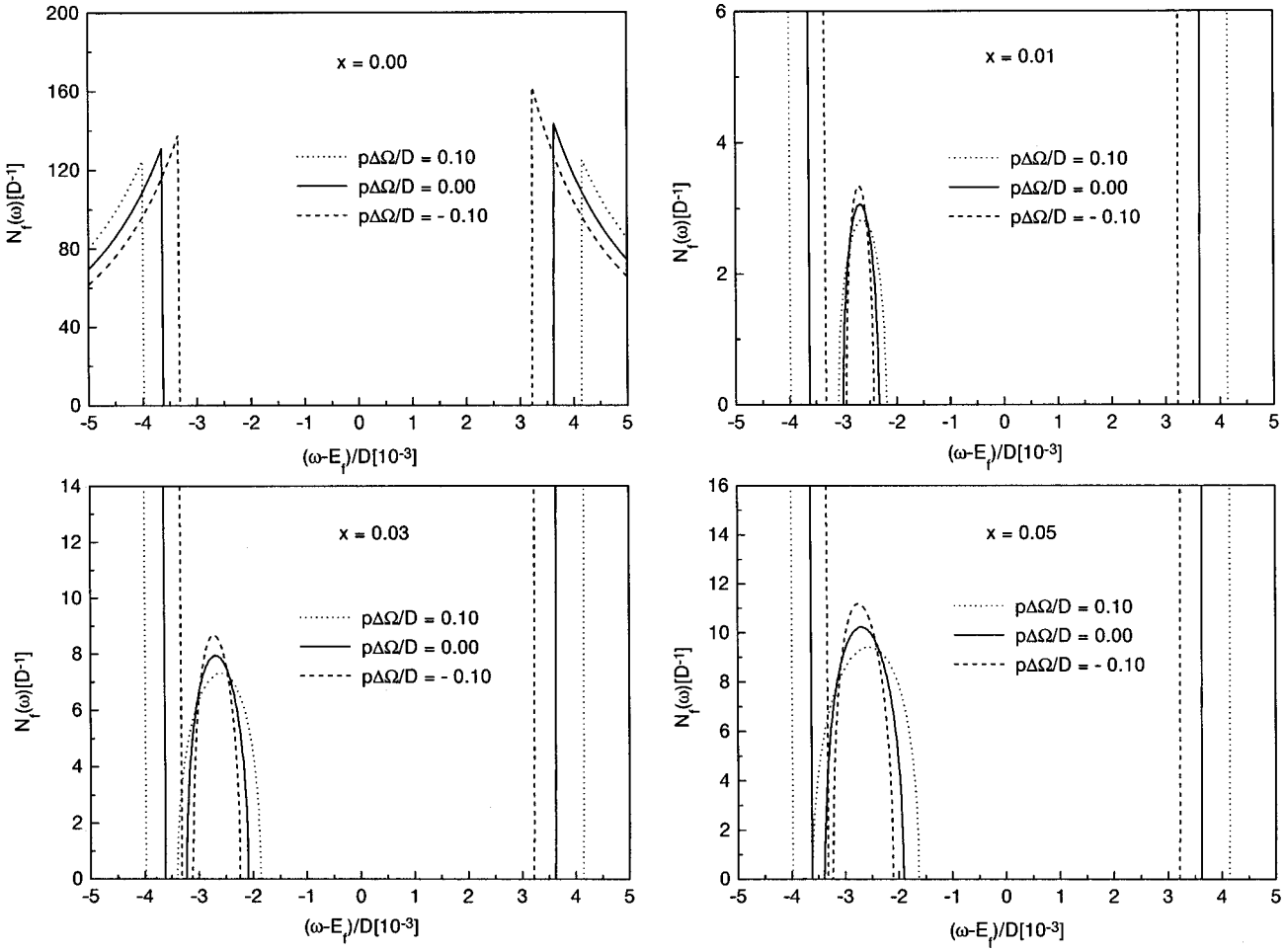

FIG. 1. Pressure influences on the *f*-DOS of Kondo insulators for impurity concentrations $x=0.00$, 0.01, 0.03, and 0.05, respectively. The parameters for numerical calculations are $V^2=0.2D^2$, $E_0=-1.2D$, and $W=0.7D$.

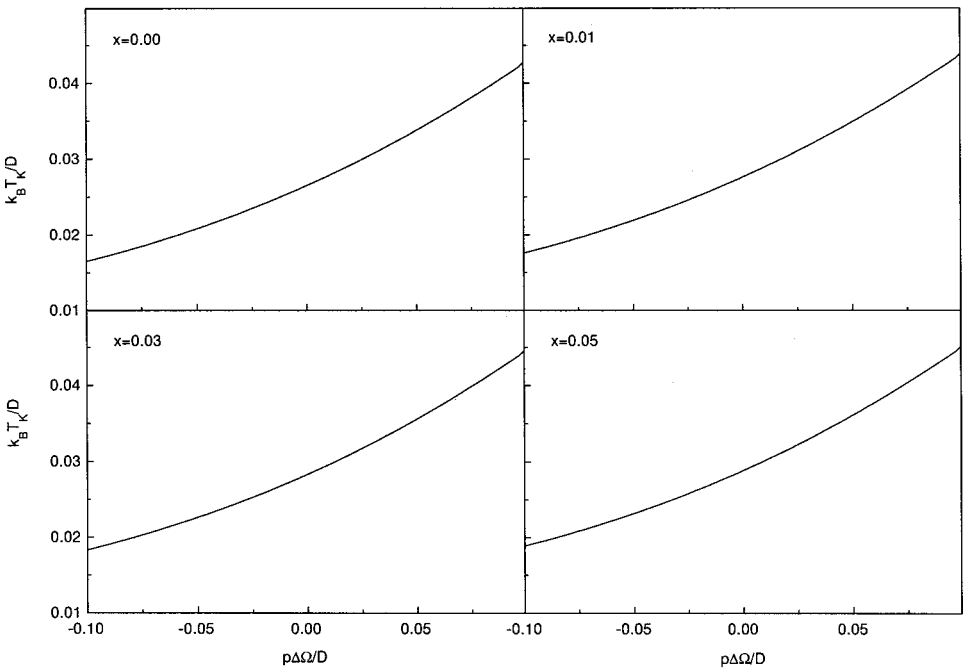

FIG. 2. Pressure dependence of the Kondo temperature T_K for two types of Kondo insulators with concentrations $x=0.00$, 0.01, 0.03, and 0.05, respectively. The parameters V^2, E_0, and W are the same as those in Fig. 1.

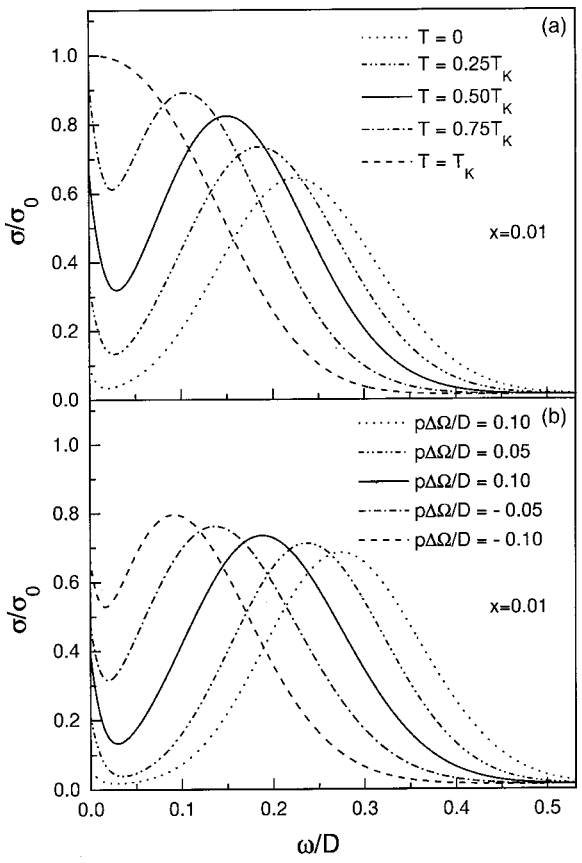

FIG. 3. The optical conductivity of Kondo insulators with impurity concentration $x=0.01$ for (a) different temperatures without pressure and (b) different pressures at $T=0.25T_K$.

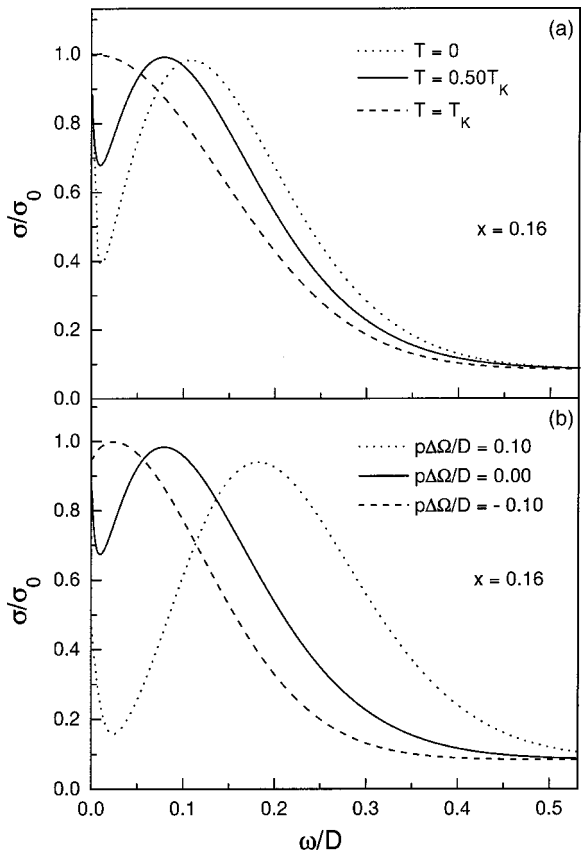

FIG. 4. The optical conductivity of Kondo insulators with impurity concentration $x=0.16$ for (a) different temperatures without pressure and (b) different pressures at $T=0.50T_K$.

The numerical results for the optical conductivity are given in Fig. 3. All the results are normalized to the conductivity $\sigma_0 \equiv \lim_{\omega\to 0} \mathrm{Re}\,\sigma(\omega)$ at Kondo temperature T_K, and both the pressure effect and the impurity effect on T_K are considered. It is explicit that there are two peaks for every curve. One is centered at $\omega=0$ presents the Drude-like peak of the conductivity at low frequencies due to the thermal activated behavior; The other peak is the IR peak due to the low-energy transitions of conduction electrons within the impurity band.[18] In Fig. 3(a), the doping concentration is fixed as $x=0.01$ without pressure. With the increasing temperature, the Drude-like peak at small frequencies increases and reaches the maximum at temperature T_K. While, due to the decoupling of *c* electrons and *f* electrons with increasing *T*, the hybridization energy gap intends to disappear and the system would transit to a metal. The IR peak displays redshift to low frequencies[18,19] and vanishes at $T=T_K$. On the other hand, in Fig. 3(b), $x=0.01$, and the temperature is fixed at $T=0.25T_K$. Under applied pressure, the *h*-type Kondo insulators (such as SmB_6 and YbB_{12}) are strikingly different from the *e*-type Kondo insulators (such as $Ce_3Bi_4Pt_3$). Pressure favors *f* configuration with smaller volume, and suppresses the hybridization gap for *h*-type Kondo insulators. Then they tend to behave like a metal more easily and the IR peak displays redshift to lower frequencies under pressure, while, the opposite effects for *e*-type Kondo insulators lead IR peak to blueshift to higher frequencies under pressure.

Though the optical conductivity indicates the temperature-dependent features of gap from the analyses stated above, the experimental results also show some temperature-independent behaviors in a large-temperature region without pressure.[18,19] After calculating on the $\sigma(\omega)$ from $x=0.01$ to $x=0.16$ [Fig. 4(a)], we find that due to the increasing doping concentration, the IR peaks are broadened and smeared out at different temperatures. All the peaks seem to be gathered [Fig. 4(a)]. When pressure is applied, for the *h*-type Kondo insulators, the IR peaks also intend to be gathered; but for the *e*-type Kondo insulators, the IR peaks can be distinguished clearly for different pressures [Fig. 4(b)]. These might imply that the impurity effect could lead to an almost temperature-independent, but pressure-dependent gap behavior for Kondo insulators, especially for the *e*-type Kondo insulators. Reasonably, that is responsible for the anomalous behavior of temperature dependence for Kondo insulators in experiments,[18,19] and also gives some suggestions on the pressure-dependent observations in further measurements.

The optical sum rule provides a formula to calculate the number of charge carrier upon the gap formation,[19]

$$\int_0^\infty \sigma(\omega,T)d\omega \propto \frac{1}{m^*}n(T), \tag{43}$$

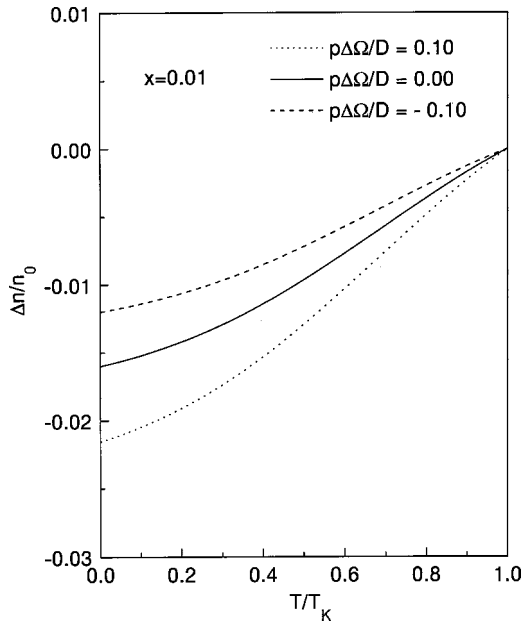

FIG. 5. Temperature dependence of the change of free electrons Δn from 0 K to T_K under various pressures, n_0 is the number of free electrons at T_K.

where m^* is the effective mass for free electrons. For Kondo insulators, *c* electrons, and *f* electrons are coupling (i.e., *c*-*f* mixing), the effective mixing strength is dependent on temperature and pressure. If we take these factors into account, Eq. (43) can be written as

$$\int_0^\infty \sigma(\omega,p,T)d\omega \propto \frac{1}{m^*}n(p,T)$$

$$= \frac{1}{m^*}[n_0(p,T_K)+\Delta n(p,T)], \tag{44}$$

where n_0 is the number of conduction electrons at $T=T_K$, and Δn the change of free electrons due to *c*-*f* mixing. Then,

$$\frac{\Delta n(p,T)}{m^*} \propto \int_0^\infty \sigma(\omega,p,T)d\omega - \int_0^\infty \sigma(\omega,p,T_K)d\omega, \tag{45}$$

where, we have used

$$\frac{n_0(p,T_K)}{m^*} \propto \int_0^\infty \sigma(\omega,p,T_K)d\omega. \tag{46}$$

For impurity concentration $x=0.01$, the results are shown in Fig. 5. In the calculation, the integral is cut at $\omega/D=1$, because only low-energy excitations near Fermi level E_F are considered, leading to a reasonable condition $\omega \leqslant D$, meanwhile, $\sigma(\omega,p,T)$ at different temperatures and pressures are almost the same at $\omega=D$. The influence by pressure is also considered for T_K. From Fig. 5, Δn is negative below T_K and *n* increases with a rise in *T*.[18] Due to the conservation of the total electrons, the depletion of conduction electron *n* (i.e., $-\Delta n$) should equal the increase of the localized electrons, that is

$$\Delta n_{local} = -\Delta n. \tag{47}$$

On the one hand, from the results above, the number of localized *f* electrons decreases with increasing *T*. The electron localization becomes weaker due to the smaller gap at enhanced temperatures. At $T=T_K$, Δn_{local} disappears, indicating the system undergoes a transition from a Kondo insulator to a heavy-fermion metal. On the other hand, to the effect of pressure, Δn_{local} for the *h*-type Kondo insulators ($\Delta\Omega<0$) is always less than the *e*-type Kondo ones ($\Delta\Omega>0$), it indicates that, at the same temperature, an *h*-type Kondo insulator can transit to a metal more easily than an *e*-type Kondo insulator under pressure. It is the same as the results of *f*-DOS. We suppose that the pressure dependent effect of the charge carrier may be observed experimentally, as the experiments of neutron scattering[5] and magnetic susceptibility[4] for the temperature dependence.

IV. CONCLUSIONS

In this paper, the pressure effects on the optical conductivity are studied by using the single-site CPA in the framework of slave-boson mean-field theory. The *f*-electron density of states (*f*-DOS), Kondo temperature T_K, and the optical conductivity are obtained in our CPA formalism for both *h*-type Kondo insulators and *e*-type Kondo insulators. It is found that impurity band emerges within the gap near the edge of the lower band, and the hybridization gap intends to disappear with increasing temperature. The system would transit to a metal. The IR peak of the optical conductivity redshifts and vanishes at $T=T_K$. At a moderate doping ($x=0.16$), the optical conductivity seems to exhibit a temperature-independent gap behavior. All these can be used to interpret the experimental results, which imply that the incoherent scattering of charge carrier within a Kondo impurity system is the crucial factor of the low-energy optical transport process.[19] On the other hand, pressure suppresses Kondo interaction and hybridization gap for a *h*-type Kondo insulator. It tends to transit to a metal more easily than an *e*-type Kondo insulator and the IR peak of the optical conductivity redshifts under pressure. Conversely, pressure promotes Kondo interaction and hybridization gap for an *e*-type Kondo insulator, and the IR peak blueshifts under pressure. The numbers of the conduction electrons and the local electrons are also discussed, which are in agreement with the results stated above. Although, there are almost no measurements on the pressure dependence of the optical conductivity, we have given some results theoretically, which might be realized in experiments before long.

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