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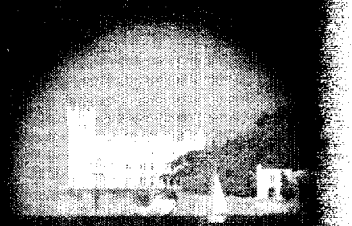

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Cheng-chung Lee (Z.Z. Li)

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EFFECTS OF PRESSURE ON DOPED KONDO INSULATORS

Cheng-chung Lee (Z.Z. Li)*
Department of Physics, Nanjing University,
Nanjing 210093, People's Republic of China†
and
The Abdus Salam International Centre for Theoretical Physics,
Trieste, Italy.

and

Wang Xu
Department of Physics, Nanjing University,
Nanjing 210093, People's Republic of China.

Abstract

The effects of pressure on the doped Kondo insulators (KI) are studied in the framework of the slave-boson mean-field theory under the coherent potential approximation (CPA). A unified picture for both electron-type KI and hole-type KI is presented. The density of states of the f-electrons under the applied pressures and its variation with the concentration of the Kondo holes are calculated self-consistently. The specific heat coefficient, the zero-temperature magnetic susceptibility as well as the low temperature electric resistivity of the doped KI under various pressures are obtained. The two contrasting pressure-dependent effects observed in the doped KI systems can be naturally explained within a microscopic model.

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*Senior Associate of the Abdus Salam ICTP.
†Permanent address.

I. INTRODUCTION

In recent years, there have been considerable amounts of works that were focused on the theories [1–5] and the experiments [6–8] of Kondo insulators (KI). Theoretically, the effects of pressure [9,10] in the KI as well as the effects of alloying [4,5] have been explored intensively. In these theories, the slave-boson mean-field approximation (SBMFA) is applied to construct the KI model and the two effects are considered separately. The incorporated effects of both the pressure and the doping have not yet been discussed theoretically.

In the present paper, we intend to investigate the effects of the pressures on the doped KI. A unified model in which the two effects are both included is introduced.

The rest of this paper is structured as follows: In Sec. II, a CPA formalism for the doped KI in the framework of SBMFA is constructed. In Sec. III, the self-consistent calculations on the f-electron's density of states (f-DOS) in the doped KI are performed numerically. The slave-boson mean-field parameters versus concentration of Kondo holes under various pressures are also computed. The effect of the Kondo holes on low-temperature specific-heat coefficient, the zero-temperature static susceptibility and their pressure dependences are given in Sec. IV. The residual and low temperature resistivities are calculated in Sec. V, where the variations of the resistivities with the applied pressures for two types of KI are demonstrated and compared with the experiments. Finally, Sec. VI contains a summary of our results.

II. DISORDER MODEL AND CPA FORMALISM

The doped Kondo insulator system considered in this paper can be considered as an alloy containing two kinds of rare-earth atoms A and B, where A (La-like) is a nonmagnetic atom without any f-electrons, and B (Ce-like, Yb-like) a magnetic atom with f-electrons. The substitution of A for B creates the missing of the f-electrons which are referred to as the Kondo holes. As an appropriate starting point for discussing doped KI, we introduce the compositional disorder into the non-degenerate Anderson lattice model with a half-filled conduction band. The random variable in the lattice point l is defined by

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

Note that the random average $\overline{\xi_l^2} = \overline{\xi_l} = x$, where x is the normalized concentration of A atoms (Kondo holes).

In the strong correlation limit: $U \to \infty$, double occupation on the B sites is forbidden, the Coleman's [11] slave-boson operator b_l is introduced in the c-f mixing term and the $U \to \infty$ Anderson lattice Hamiltonian can be written in slave-boson formalism as

$$\begin{aligned} H = & \sum_{\mathbf{k}\sigma}[\varepsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + (-E_0) f^\dagger_{\mathbf{k}\sigma} f_{\mathbf{k}\sigma}] + \sum_{i\sigma} \xi_i (E_L + E_0) f^\dagger_{i\sigma} f_{i\sigma} \\ & + V \sum_{i\sigma} (1-\xi_i)(b_i f^\dagger_{i\sigma} c_{i\sigma} + c^\dagger_{i\sigma} f_{i\sigma} b^\dagger_i) + \sum_i (1-\xi_i)\lambda_i (\sum_\sigma f^\dagger_{i\sigma} f_{i\sigma} + b^\dagger_i b_i - 1), \end{aligned} \tag{2}$$

where a constraint due to infinite-U

$$\sum_\sigma f^\dagger_{i\sigma} f_{i\sigma} + b^\dagger_i b_i = 1 \qquad \text{for } i \in B, \tag{3}$$

is added with the Lagrange multiplier λ_i. This constraint prevents the double occupancy of f-level on the B sites. In Eq. (2), $(-E_0)$ is the energy of f electrons on magnetic (B) atoms, and E_L represents the f level on Kondo holes (nonmagnetic A atoms).

Now let us introduce the total volume operator. In pure Kondo-lattice system, such as SmB_6, YbB_{12}, $Ce_3Bi_4Pt_3$ etc., the most typical valence-fluctuation ions Ce, Sm, Eu, and Yb can exist in two valence states [1]: 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:

$$\begin{cases} f^{n+1}(j,+m) \rightleftharpoons f^n(j=0) + e^-(j,m) & \text{for Ce and Eu} \\ f^{n-1}(j,-m) \rightleftharpoons f^n(j=0) + h^+(j,m) & \text{for Sm and Yb} \end{cases} \tag{4}$$

In terms of Coleman's slave boson technique [11],

$$b_l^\dagger \mid 0\rangle_l = \mid f^n : j=0\rangle_l, \tag{5}$$

$$f^\dagger \mid 0\rangle_l = \mid f^{n\pm1} : j, \pm m\rangle_l, \tag{6}$$

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 an electron e^- for Ce, Eu, and becomes a hole h^+ for Sm, Yb, 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 [9]

$$\Omega_t = \sum_l \Omega_l = \sum_l [b_l^\dagger b_l \Omega_0 + (1 - b_l^\dagger b_l)\Omega_1], \tag{7}$$

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

In the case of doping, we can express the total volume operator of doped KI system in terms of random variable ξ_l as

$$\Omega_t = \sum_l \{\xi_l \Omega_L + (1-\xi_l)[b_l^\dagger b_l \Omega_0 + (1 - b_l^\dagger b_l)\Omega_1]\}, \tag{8}$$

where Ω_L is the cell volume of a Kondo-hole site (with La-like ions), Ω_0 and Ω_1 are the cell volumes of a B site 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 (3) 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 [5]

$$\begin{aligned} H_{MF} = & \sum_{\mathbf{k}\sigma} [(\varepsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + E_f f_{\mathbf{k}\sigma}^\dagger f_{\mathbf{k}\sigma}) + rV(f_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + c_{\mathbf{k}\sigma}^\dagger f_{\mathbf{k}\sigma})] \\ & + (1-x)N_s\lambda(r^2-1) + \sum_{l\sigma} [\varepsilon_L f_{l\sigma}^\dagger f_{l\sigma} - rV(f_{l\sigma}^\dagger c_{l\sigma} + c_{l\sigma}^\dagger f_{l\sigma})], \end{aligned} \tag{9}$$

where $E_f = E_0 + \lambda$ and $\varepsilon_L = E_L - E_0$ are the renormalized f-level of the magnetic (B) atoms and the Kondo holes (A atoms), respectively. Because a Kondo hole doping will lead to a very strong scattering, $E_L \to \infty$, so that $\varepsilon_L \to \infty$, we have to solve the disorder slave-boson mean-field

Hamiltonian (9) for arbitrary concentrations of the Kondo holes by means of a nonperturbative approach— the coherent potential approximation (CPA).

The coherent potential should be assumed as a 2×2 matrix: [4]

$$S(\omega,\ x) = \begin{pmatrix} S_{cc} & S_{cf} \\ S_{fc} & S_{ff} \end{pmatrix}. \tag{10}$$

The effective medium Hamiltonian can be written in the matrix form:

$$\overline{H} = \sum_{\mathbf{k}\sigma} \begin{pmatrix} c^{\dagger}_{\mathbf{k}\sigma} & f^{\dagger}_{\mathbf{k}\sigma} \end{pmatrix} \begin{pmatrix} \varepsilon_{\mathbf{k}} + S_{cc} & S_{cf} \\ S_{fc} & E_f + S_{ff} \end{pmatrix} \begin{pmatrix} c_{\mathbf{k}\sigma} \\ f_{\mathbf{k}\sigma} \end{pmatrix} + N_s\lambda(1-x)(r^2-1), \tag{11}$$

where N_s is the number of unit cell in the system. In Bloch representation, the matrix of the medium Green's function (GF) is determined by $(\omega - \overline{H})^{-1}$ in the space of basis vector $(c^{\dagger}_{\mathbf{k}\sigma},\ f^{\dagger}_{\mathbf{k}\sigma})$ and reads

$$\overline{G}(\omega,\ \mathbf{k}) = \frac{1}{B_{\mathbf{k}}} \begin{pmatrix} \omega - E_f - S_{ff} & S_{cf} \\ S_{fc} & \omega - \varepsilon_{\mathbf{k}} - S_{cc} \end{pmatrix}, \tag{12}$$

with

$$B_{\mathbf{k}} = (\omega - \varepsilon_{\mathbf{k}} - S_{cc})(\omega - E_f - S_{ff}) - S_{cf}S_{fc}. \tag{13}$$

From Eq. (12), we obtain the average site GF of the effective medium

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

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 the 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 [12], this requirement is equivalent to a self-consistent equation in single-site CPA

$$xt_A + (1-x)t_B = 0, \tag{15}$$

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

$$t_{A(B)} = V_{A(B)}[1 - F(\omega)V_{A(B)}]^{-1}, \tag{16}$$

which can be determined from

$$\begin{aligned} H_{MF} - \overline{H} &= \sum_{l\sigma} \begin{pmatrix} c^{\dagger}_{\mathbf{k}\sigma} & f^{\dagger}_{\mathbf{k}\sigma} \end{pmatrix} \begin{pmatrix} -S_{cc} & (1-\xi_l)rV - S_{cf} \\ (1-\xi_l)rV - S_{fc} & \xi_l\varepsilon_L - S_{ff} \end{pmatrix} \begin{pmatrix} c_{\mathbf{k}\sigma} \\ f_{\mathbf{k}\sigma} \end{pmatrix} \\ &= \sum_{l\sigma} \begin{pmatrix} c^{\dagger}_{\mathbf{k}\sigma} & f^{\dagger}_{\mathbf{k}\sigma} \end{pmatrix} \widehat{V} \begin{pmatrix} c_{\mathbf{k}\sigma} \\ f_{\mathbf{k}\sigma} \end{pmatrix}, \end{aligned} \tag{17}$$

where

$$\widehat{V} \equiv \begin{pmatrix} -S_{cc} & (1-\xi_l)rV - S_{cf} \\ (1-\xi_l)rV - S_{fc} & \xi_l\varepsilon_L - S_{ff} \end{pmatrix}. \tag{18}$$

For $\xi_l = 1$,we have

$$\widehat{V} = V_A = \begin{pmatrix} -S_{cc} & -S_{cf} \\ -S_{fc} & \varepsilon_L - S_{ff} \end{pmatrix}, \tag{19}$$

and for $\xi_l = 0$, we have

$$\widehat{V} = V_B = \begin{pmatrix} -S_{cc} & rV - S_{cf} \\ rV - S_{fc} & -S_{ff} \end{pmatrix}. \tag{20}$$

Substituting Eqs. (19) and (20) into (15), and taking $\varepsilon_L \to \infty$ (because $E_f \ll \varepsilon_L$, $E_L \to \infty$) to ensure zero f-electron on the A-sites, after some algebraic manipulations, we can find a analytic solution of the coherent potential

$$S(\omega,\ x) = \begin{pmatrix} 0 & rV \\ rV & S_{ff} \end{pmatrix}, \tag{21}$$

where only the matrix element S_{ff} is unknown. At the same time, the self-consistent CPA equation (15) can be simplified as

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

Then, the average site GFs are expressed as

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

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

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

The parameters of SB, r and λ, can be determined by the extreme values of the grand canonical free enthalpy's variations. The grand canonical free enthalpy of the doped KI system under pressure is

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

where

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

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

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

From the variation with respect to λ

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

we get the equation including parameter r

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

And the same procedure to r

$$0 = \frac{\delta K}{\delta r} = \langle \frac{\partial H_{eff}}{\partial r} \rangle_T$$
$$= V \sum_{k\sigma} (\langle c^\dagger_{k\sigma} f_{k\sigma} \rangle_T + \langle f^\dagger_{k\sigma} c_{k\sigma} \rangle_T) + 2(1-x) N_s r(\lambda - p\Delta\Omega). \tag{31}$$

implies the another equation:

$$(1-x) r(\lambda - p\Delta\Omega) = -2V \{ \frac{1}{N_s} \sum_{k\sigma} \langle f^\dagger_{k\sigma} c_{k\sigma} \rangle_T \}$$
$$= \frac{2V}{\pi} \int_{-\infty}^{\infty} d\omega f(\omega - \mu) \mathrm{Im} F_{fc}(\omega + i0^+). \tag{32}$$

The chemical potential μ can be obtained from the conservation of the total number of the particles:

$$N_t = -\frac{\partial K}{\partial \mu} = (2-x) N_s, \tag{33}$$

where we have assumed that there is only one conduction electron per site for the doped KI system. Eq. (33) can be rewritten as

$$(2-x) = -\frac{2}{\pi} \int_{-\infty}^{\infty} d\omega f(\omega - \mu) \mathrm{Im}[F_{cc}(\omega + i0^+) + F_{ff}(\omega + i0^+)]. \tag{34}$$

Within SBMFA, the averaged cell-volume is

$$\overline{\Omega_l} = x\Omega_L + (1-x)[\Omega_0 + (1-r^2)\Delta\Omega], \tag{35}$$

where

$$\Delta\Omega \equiv \Omega_1 - \Omega_0. \tag{36}$$

Since the pressure always decreases the averaged cell-volume $\overline{\Omega_l}$, for the electron-type KI where $\Delta\Omega > 0$, in this case the pressure will lead to the increasing of r^2. For the hole-type KI, an opposite effect exists since $\Delta\Omega < 0$.

Eqs. (22), (25), (30), (32), (34), and (35) constitute a set of self-consistent equations. These equations are not only fundamental to determine the coherent potential $S_{ff}(\omega, x)$, the SB parameters r and λ, the chemical potential μ, and the Kondo temperature T_k of the doped KI during different pressures, but also powerful for calculating the electronic DOS of the heavy fermion alloys with arbitrary Kondo-hole concentrations under various pressures.

III. THE f-DOS IN DOPED KI

The f-electron density of states (f-DOS) in doped Kondo insulators under pressure is defined by the imaginary part of the effective-medium GF, $F_{ff}(\omega)$. The f-DOS per magnetic (B) atom can be written as

$$N_f(\omega,\ p\Delta\Omega,\ x) = -\frac{1}{\pi(1-x)} \mathrm{Im} F_{ff}(\omega + i0^+), \tag{37}$$

where $F_{ff}(\omega)$ can be calculated self-consistently from Eqs. (22), (25), (30), and (32) by numerical method. In the calculations, the unperturbed DOS of conduction electrons, $N_0(\omega)$, is assumed as

$$N_0(\omega) = \begin{cases} \frac{1}{2D} & \text{for } |\omega| < D \\ 0 & \text{for } |\omega| > D \end{cases}, \tag{38}$$

where D is the half-width of the conduction band.

The numerical results of f-DOS are shown in Fig. 3. The SB parameters r^2, T_K, E_f and μ can also be solved numerically from self-consistent equations, and are shown in Figs. 1 and 2. T_K is the Kondo temperature, it is dependent on pressure, but not on the doping concentration x. The effect of pressure increases Kondo interaction and hybridization for electron-type KI and, on the contrary, suppresses them for the hole-type KI. As to the effects of doping, adding Kondo holes into the KI leads to an impurity band, and the band is broadened with increasing the Kondo-hole concentration x [5]. In the moderate doping concentration when $x \geq 0.15$, the gap will be gradually smear out, and instead, there will occur a "two-peak" psudo-gap structure. It is easy to see that upon doping the system will change from a Kondo insulator into a heavy-fermion metal [5]. From Fig. 3, one can easily discover that at the doping concentration $x = 0.15$, where the ambient-pressure gap of the system becomes very small, the gap of the hole-type KI under the applied pressure can be depressed to zero, and the KI system undergoes a pressure-induced transition from an insulator to a metal. This I-M transition presents the incorporated effect of both the doping and the pressure in the hole-type KI system, which is accordance with the experimental observations in the SmB_6 (h-KI) [14,15] .

IV. THERMALDYNAMICAL QUANTITIES

In this section we shall calculate the low-temperature specific-heat coefficient and the zero-temperature magnetic susceptibility of the doped KI under various pressures. Although, to the best of our knowledge, there is no experimental results concerning the pressure influences of the specific-heat coefficient and the magnetic susceptibility on the doped Kondo insulators, we would like to make some theoretical predictions here.

(a) Specific-heat coefficient of the doped KI: In the low-temperature region, the main contribution of the specific heat comes from f-electron near Fermi level, and the specific heat coefficient of the doped KI can be written in terms of f-DOS as

$$\gamma(T,\ p\Delta\Omega,\ x) = \frac{1}{2}k_B^2\beta^3 \int_{-\infty}^{\infty} d\omega(\omega-\mu)^2 N_f(T,\ p\Delta\Omega,\ x)\mathrm{sech}^2[\frac{\beta(\omega-\mu)}{2}], \tag{39}$$

where $\beta = 1/k_BT$, and $N_f(T, p\Delta\Omega, x)$ is the f-DOS of the alloying KI. The numerical results are given in Fig. 4, the case of $x = 0$, γ-T curves vanishes at $T = 0$ due to the existence of real gaps in the excitation spectrum [5,9]. On the one hand, the substitution of La for Ce gradually smears out the gap, and leads the system to a disordered-induced metallic phase, so for moderate doping ($x \geq 0.15$) the γ-T curves behave like a heavy fermion metal with a pseudo-gap, as shown in Fig. 4 [5]. On the other hand, the pressure promotes the specific-heat coefficient values for the hole-type KI and, on the contrary, suppresses the values for the electron-type KI.

(b) Zero-temperature magnetic susceptibility: The static magnetic susceptibility of the pure KI can be expressed as

$$\chi = \chi_{V.V.} + \chi_{Pauli}, \tag{40}$$

where $\chi_{V.V.}$ is an interband Van Vleck contribution to the susceptibility and is of order $g_L^2\mu_B^2/4D$ as pointed out by Riseborough [2], and μ_B is the Bohr magneton, g_L the Lande factor of f-electrons. χ_{Pauli} represents the Pauli spin susceptibility [3].

The $T = 0$ Pauli susceptibility for the doped KI can be obtained from the well-known formula

$$\chi_{Pauli}(T = 0,\ x) = \frac{1}{4} g_L^2 \mu_B^2 N_f(\mu,\ x). \tag{41}$$

After adding a Van Vleck origin constant contribution to the susceptibility, we get the numerical results in the limit of small Kondo hole concentrations. In Fig. 5, the influence of pressure on the susceptibility is shown evidently and directly, and in the limit $x \to 0$, $\chi_{Pauli} \sim \sqrt{x}$, which shows the magnetic susceptibility of the doped KI goes up with increase in Kondo hole concentration x as obtained from the experiment [8]. The above theoretical predictions may be useful for the further experimental studies on the pressure-dependent properties of the doped KI systems.

V. LOW-TEMPERATURE RESISTIVITY

(a) Residual resistivity at $T = 0$: Once the effective medium $S(\omega, x)$ is found, we can get the conductivity of our system from Kubo formula [5]

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

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

$$\overline{G}_{cc}(\mathbf{k},\ p,\ \omega) = \frac{\omega - E_f - S_{ff}}{(\omega - \varepsilon_{\mathbf{k}})(\omega - E_f - S_{ff}) - (rV)^2}, \tag{43}$$

is the matrix element of the effective-medium GF for the conduction electrons. At zero temperature [5],

$$\sigma(T = 0,\ x) = \frac{2e^2 v_F^2}{3\pi\hbar^2\Omega} \sum_{\mathbf{k}} [\mathrm{Im}\overline{G}_{cc}(\mathbf{k},\ p,\ \mu + i0^+)]^2, \tag{44}$$

where

$$\mathrm{Im}\overline{G}_{cc}(\mathbf{k}, p, \mu + i0^+) = \mathrm{Im}[\frac{\mu - E_f - S_{ff}(\mu + i0^+)}{(\mu - \varepsilon_{\mathbf{k}})(\mu - E_f - S_{ff}(\mu + i0^+)) - (rV)^2}]. \tag{45}$$

The residual resistivity $\rho(T = 0,\ p,\ x) = 1/\sigma(T = 0, p, x)$ can be computed from Eq. (45). Numerical results of residual resistivity with dilute Kondo hole concentrations under various pressures is shown in Fig. 6. It is very clear that, for the electron-type KI, the residual resistivity increases with increasing pressure, and for the hole-type KI, the residual resistivity decreases with increasing pressure. This result is in agreement with the pressure-dependent experiments of resistivity for two types of KI by Thompson et al. [13], Beille et al. [14] and Cooley et al. [15]. Therefore, our theory provides a unified interpretation at the first time on the pressure-dependent residual resistivity for the Kondo Insulators of both two types.

(b) Low-temperature resistivity: At low temperature, the total conductivity σ_t can be expressed as

$$\sigma_t = \sigma_1 + \sigma_2, \tag{46}$$

where, σ_1 is from the temperature effects of Kondo hole scattering, σ_2 is the contribution of the SB fluctuations around the MF at finite temperatures.

From Eq. (42), we can get the conductivity at the finite temperatures,

$$\sigma_1(T,\ p,\ x) = \frac{2e^2v_F^2}{3\pi\hbar^2\Omega}\int_{-\infty}^{\infty} d\omega[-\frac{\partial f}{\partial\omega}]\sum_{\mathbf{k}}[\mathrm{Im}\overline{G}_{cc}(\mathbf{k},\ p,\ \omega+i0^+)]^2$$
$$= \sigma_1(0,\ p,\ x) + \sigma_1(T,\ p,\ x), \tag{47}$$

where $\sigma_1(0,\ p,\ x)$ is the zero-temperature residual resistivity given above.

After direct calculation, we get $\sigma_1(T,\ p,\ x)$ at the limit $x \to 0$ as

$$\sigma_1(T,p,x \to 0) = \sigma_1(0,\ p,\ x \to 0)(1 + g(x)(\frac{k_BT}{D})^2), \tag{48}$$

where $g(x)$ is a function of x, independent of pressure,

$$g(x) = \frac{\pi^2}{3}[32(1-x)(1-2x-\frac{3-2x}{(9-8x)^2})]. \tag{49}$$

Based on Ref.[9], σ_2 can be written as

$$\sigma_2 = \frac{16e^2\hbar}{3m^*D}(\frac{r^2}{\eta^2})\exp(-\frac{r^2V^2}{Dk_BT}), \tag{50}$$

where m^* is the effective mass, η^2 represents the slave boson fluctuation which is proportional to the temperature [9]. $\sigma_t = \sigma_1 + \sigma_2$, then

$$\rho_t(T,\ p,\ x \to 0) = \frac{1}{\sigma_1(T=0,\ p,\ x \to 0) + \sigma_2(T,\ p,\ x \to 0)}. \tag{51}$$

The numerical results of the low temperature resistivity under the applied pressure have been given in Fig. 7. Fig. 7 shows that in the dilute Kondo hole concentration ($x = 0.01$), the low-T resistivity for the electron-type KI enhances with the increasing of the pressure, which corresponds to the observation in the $Ce_3Bi_4Pt_3$ [13]; For the hole-type KI, the resistivity decreases with the increasing of the applied pressure in agreement with the experiments in the SmB_6 [14,15]. Therefore, the two opposite pressure-dependent effects on resistivity observed in e-KI and h-KI can be naturally derived from a unified picture.

VI. CONCLUSIONS

In this paper, the pressure effects on the doped KI are studied by using the single-site CPA in the framework of the slave-boson mean-field theory. The f-electron density of states in the whole concentration range under various pressures is calculated self-consistently in our CPA formalism for both e-type and h-type KI. It is found that as the applied pressure increases, the Kondo interaction and hybridization gap increase for the e-type KI, and on the contrary, they decrease for the h-type KI. It is also shown that with a small concentration of Kondo holes ($x \ll 0.15$), an impurity band appears in the middle of the hybridization gap. As the concentration increases, this impurity band grows wider and higher and gradually merges with the lower and upper hybridized bands. The system gradually changes from an insulator to a heavy fermion metal as the gap disappears. Our numerical results of the f-DOS shown in Fig. 3 also indicate that at the concentration $x = 0.15$, where the zero-pressure gap has already been depressed to a very small value, the gap will decrease to zero with the increasing of the applied pressure for the hole-type KI. This means that, in the doped KI system, the applied pressure favors the hole-type KI to change from an insulator into a metal, which is confirm by the experiments in the SmB_6. Our theoretical result on the low-T resistivity in the doped KI systems provide a unified explanation on the two opposite pressure-dependent effects observed in Ce-based and Sm-based compounds at the first time.

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Figure Captions

FIG. 1. Alloying effects on the mean-field parameters of the doped KI under various pressures. Here x is the concentration of Kondo holes. The parameters for the numerical calculations are chosen as: $V^2 = 0.2D^2$, $E_f = 1.2D$.

FIG. 2. Pressure dependence of the Kondo temperature T_K for both two types of KI.

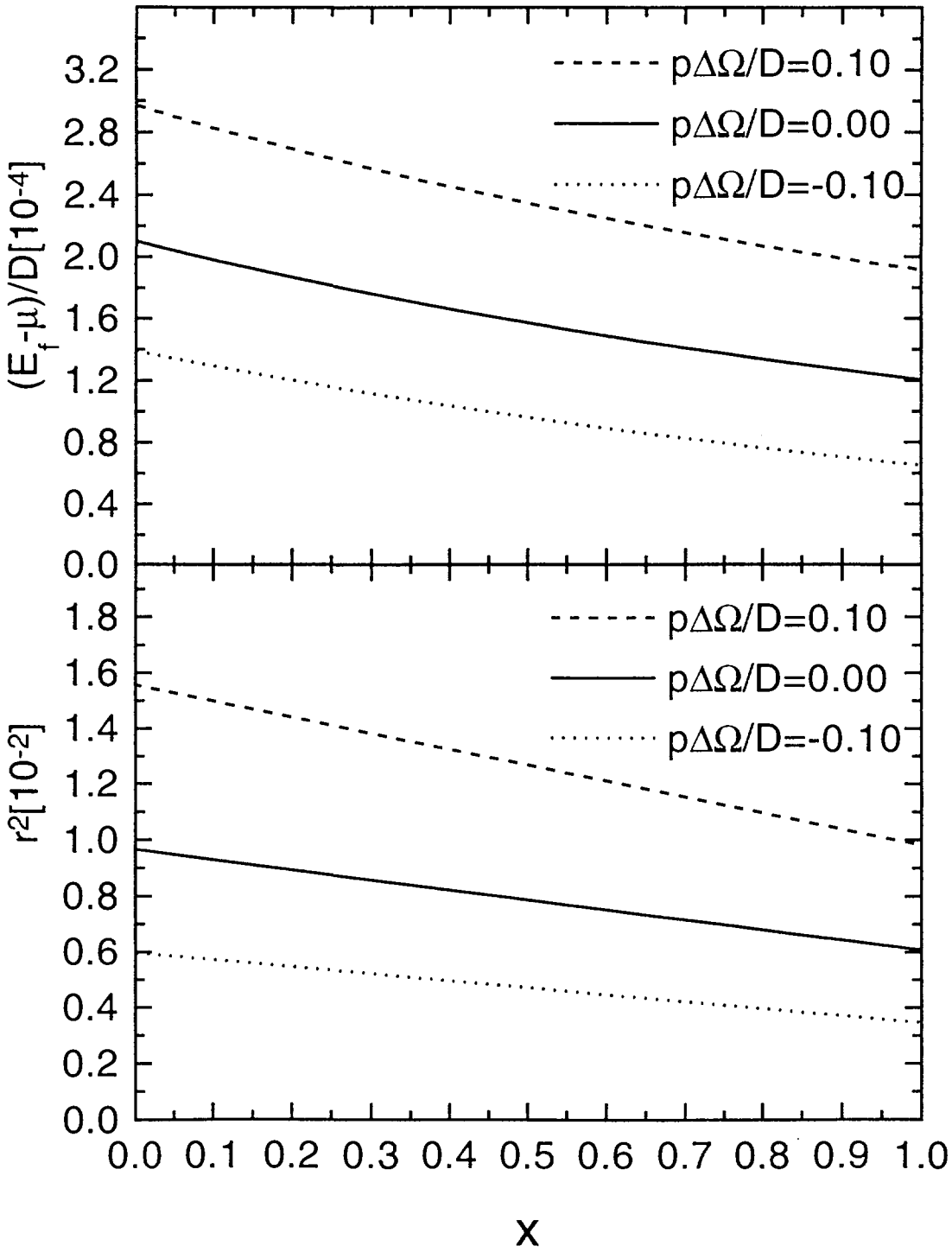
FIG. 3. Pressure influences on the f-DOS of the doped KI, respectively, for $x = 0$, $x = 0.01$, $x = 0.10$, $x = 0.15$, $x = 0.30$, and the f-DOS on Fermi level which varies with the Kondo-hole concentrations x. E_f and V are chosen as in Fig. 1.

FIG. 4. Specific heat coefficient of the doped KI, at various pressures for $x = 0$, $x = 0.05$, $x = 0.20$, and $x = 0.40$, respectively, where $\gamma_u = k_B^2/D$.

FIG. 5. Pressure dependence of magnetic susceptibility at $T = 0$ for small Kondo-hole concentrations, the necessary parameters are chosen as in Fig. 1, and $\chi_u = \mu_B^2/D$.

FIG. 6. Residual resistivity versus scaled pressures, for the dilute concentrations of $x = 0.01$ and $x = 0.05$, where $\rho_u = 3\pi\hbar^2 D^2 \Omega_c / 2e^2 v_F^2$.

FIG. 7. Pressure effects of the finite temperature resistivity with dilute Kondo-hole concentration ($x = 0.01$) for the hole-type KI and the electron-type KI, respectively.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pΔΩ/D=0.00
pΔΩ/D=-0.10
(E_f-μ)/D[10^-4]
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2.8
2.4
2.0
1.6
1.2
0.8
0.4
0.0
pΔΩ/D=0.10
pΔΩ/D=0.00
pΔΩ/D=-0.10
r^2[10^-2]
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0
X

Fig.1

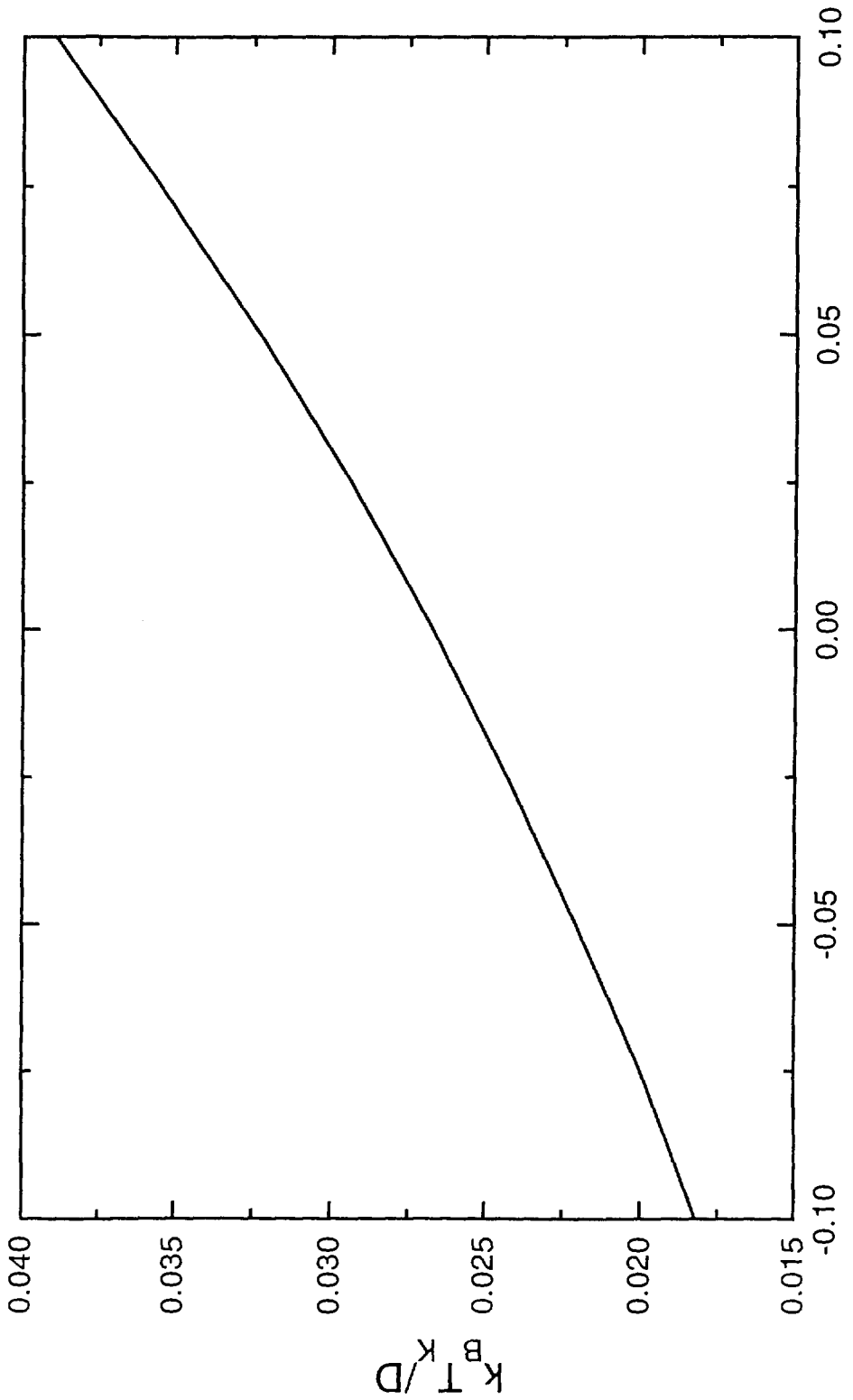
0.040
0.035
0.030
0.025
0.020
0.015
$k_B T_K/D$
-0.10
-0.05
0.00
0.05
0.10
$p\Delta\Omega/D$

Fig.2

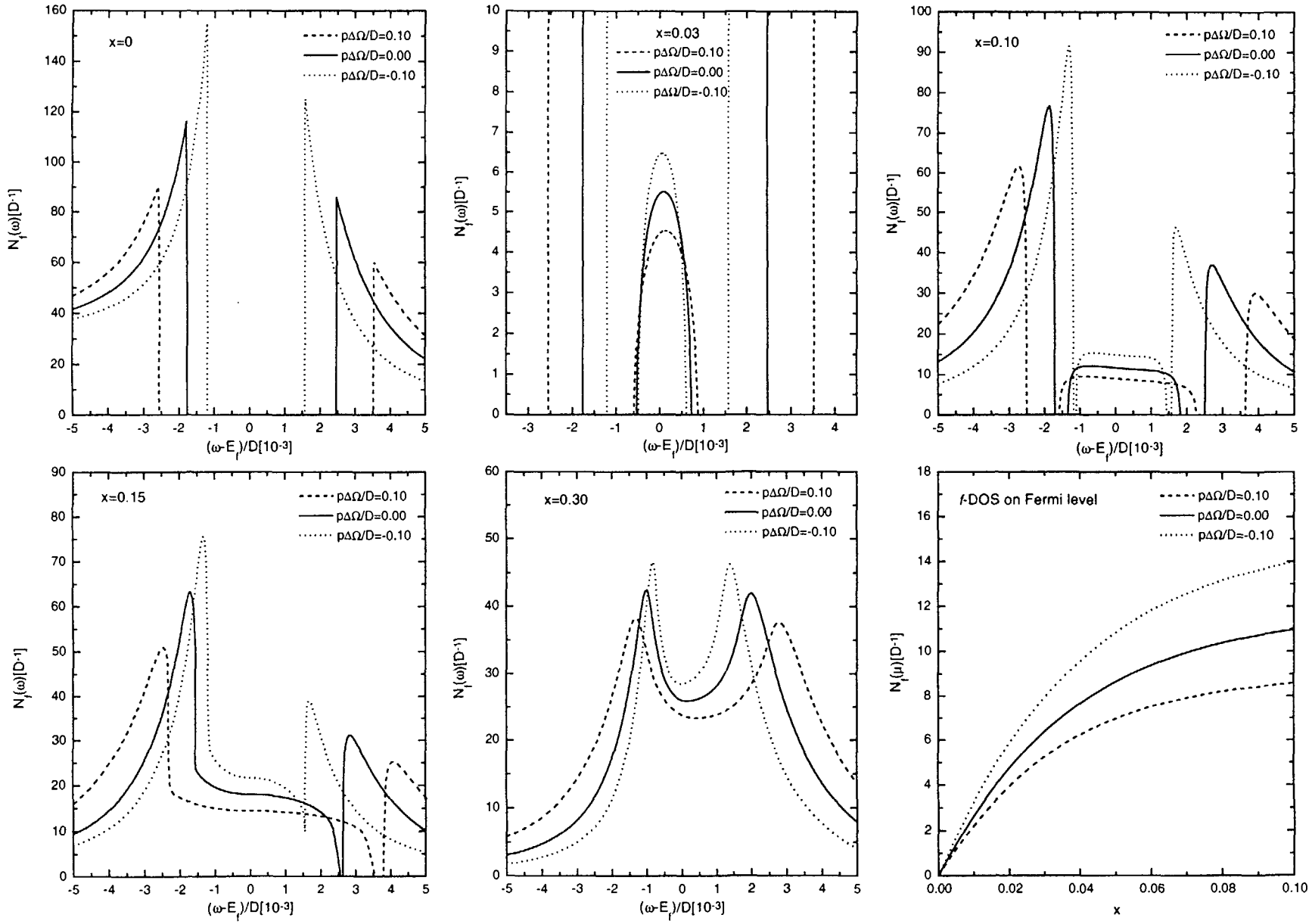
x=0
x=0.03
x=0.10
x=0.15
x=0.30
pΔΩ/D=0.10
pΔΩ/D=0.00
pΔΩ/D=-0.10
N_f(ω)[D^-1]
(ω-E_f)/D[10^-3]
f-DOS on Fermi level
N_f(μ)[D^-1]
x

Fig.3

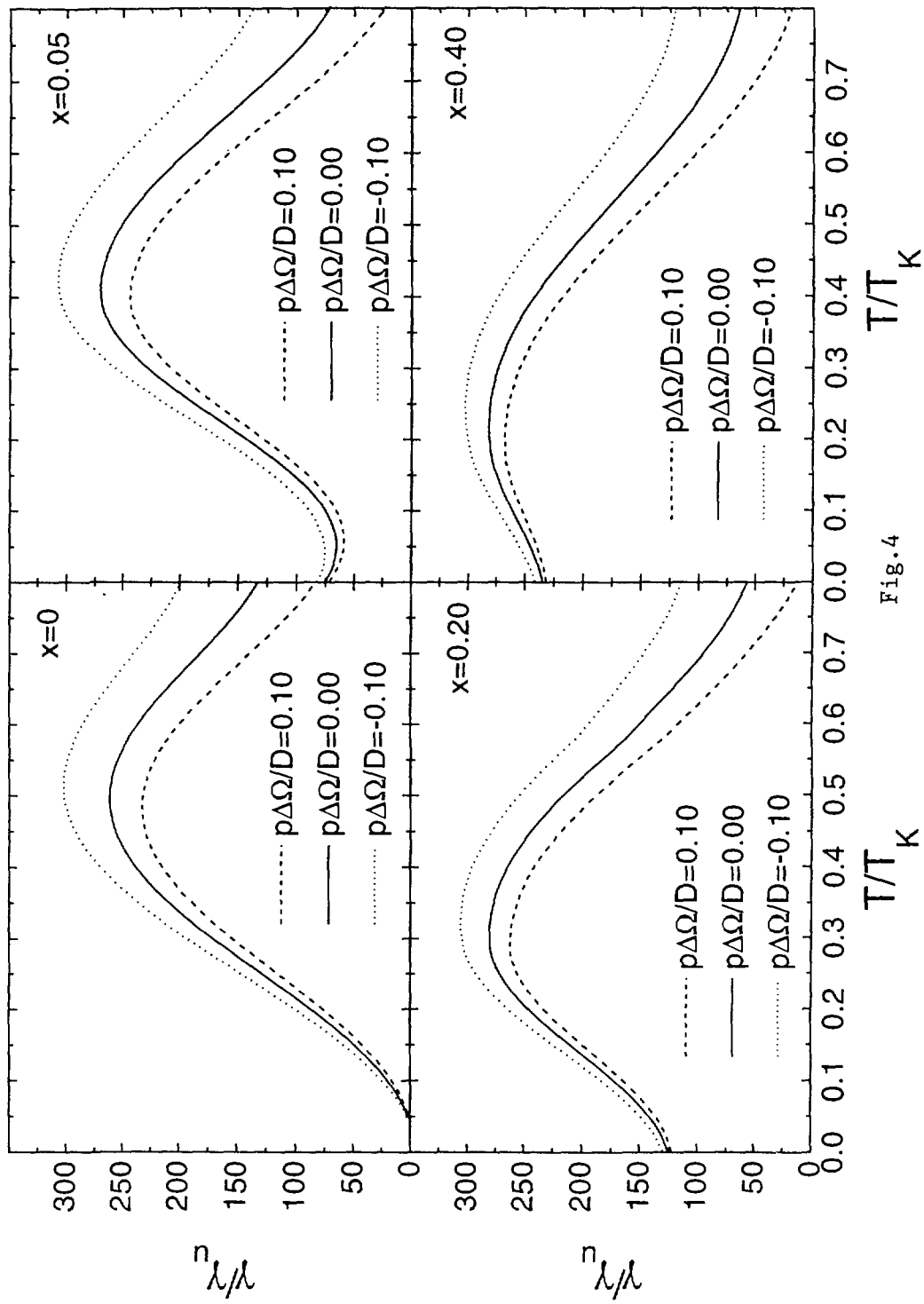
x=0
x=0.05
x=0.20
x=0.40
pΔΩ/D=0.10
pΔΩ/D=0.00
pΔΩ/D=-0.10
χ/χ_u
T/T_K
0
50
100
150
200
250
300
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7

Fig.4

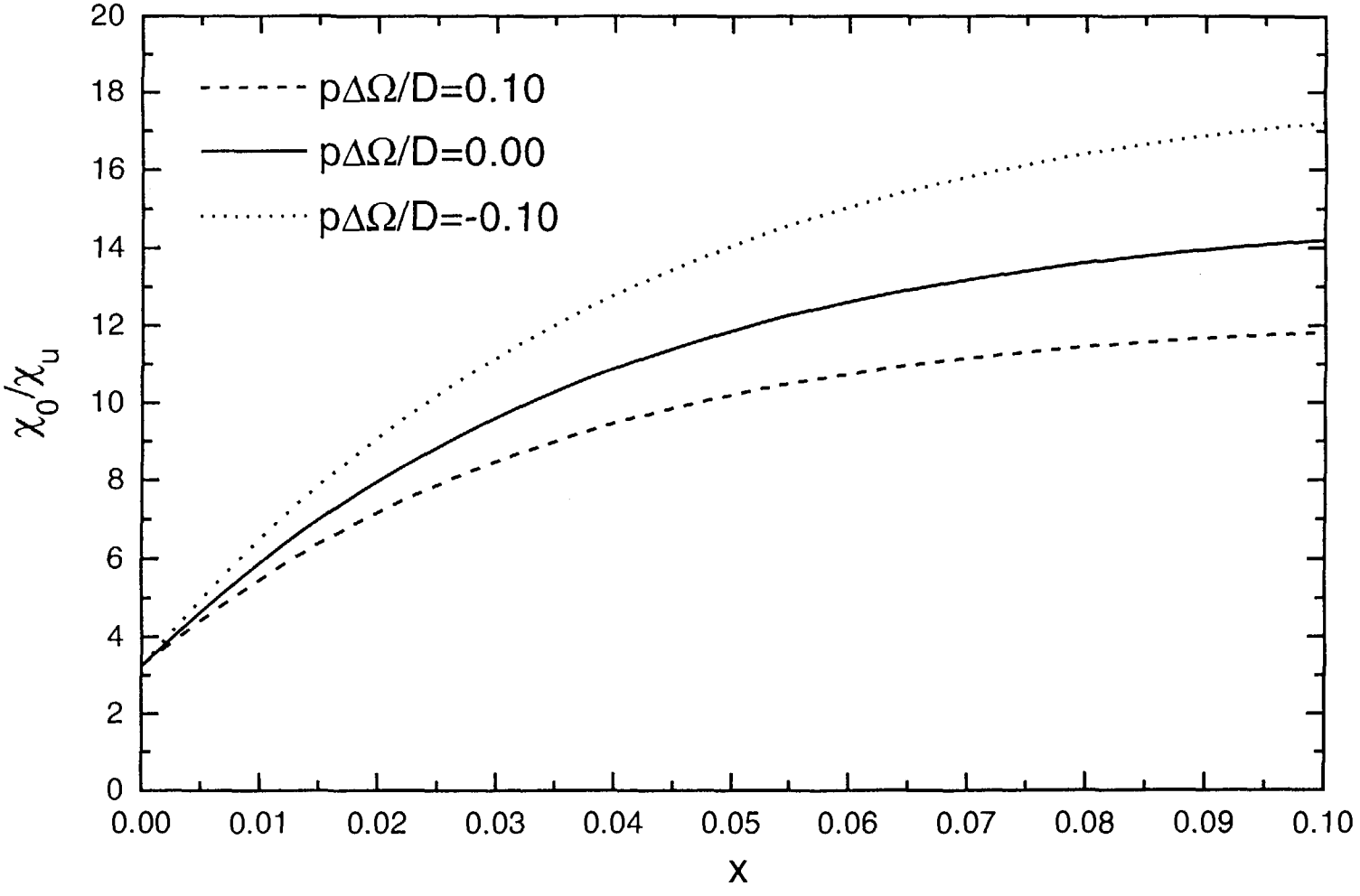
20
18
16
14
12
10
8
6
4
2
0
0.00
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
0.10
X
χ_0/χ_u
pΔΩ/D=0.10
pΔΩ/D=0.00
pΔΩ/D=-0.10

Fig.5

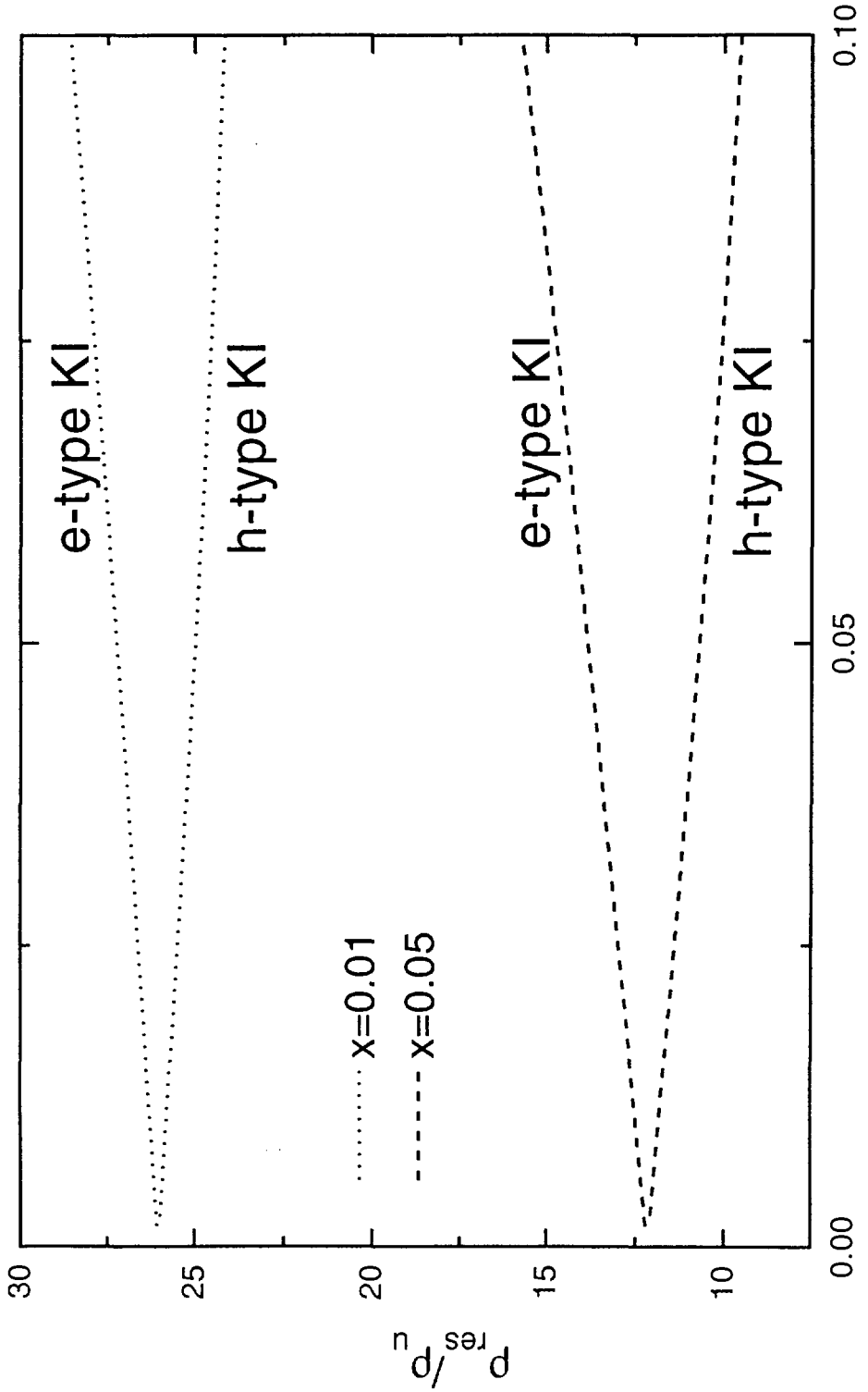
e-type KI
h-type KI
e-type KI
h-type KI
x=0.01
x=0.05
30
25
20
15
10
0.00
0.05
0.10
ρ_{res}/ρ_u
$p|\Delta\Omega|/D$

Fig.6

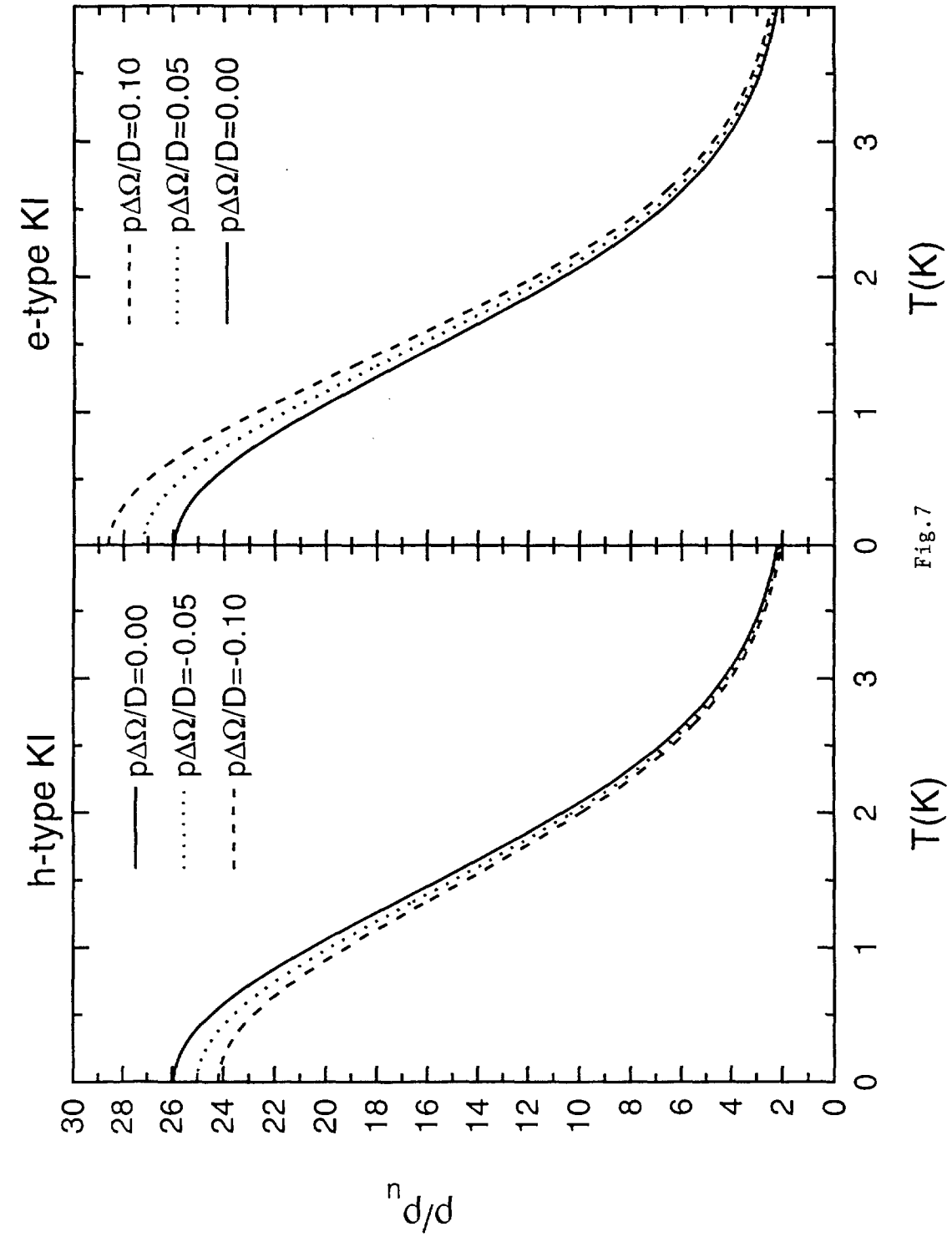
e-type KI
h-type KI
pΔΩ/D=0.10
pΔΩ/D=0.05
pΔΩ/D=0.00
pΔΩ/D=0.00
pΔΩ/D=-0.05
pΔΩ/D=-0.10
ρ/dρ
T(K)
T(K)

Fig.7