On the residual magnetoresistivities of heavy-fermion alloys

1994 J. Phys.: Condens. Matter 6 2957

(http://iopscience.iop.org/0953-8984/6/15/018)

J. Phys.: Condens. Matter 6 (1994) 2957–2964. Printed in the UK

On the residual magnetoresistivities of heavy-fermion alloys

Chun Chen and Zheng-Zhong Li
Department of Physics, Nanjing University, Nanjing, 210008, People's Republic of China

Received 2 September 1993, in final form 1 December 1993

Abstract. Based on the two-conduction-band periodic Anderson model, including the effects of Kondo holes and conduction band impurities, the residual magnetoresistivities (MRs) of heavy-fermion (HF) alloys have been calculated in the single-site coherent-potential approximation. The strong correlation of HF systems is treated by the slave-boson technique. Our results show that only negative residual MRs can be obtained in 'pure' Kondo-hole alloys and only positive residual MRs can be obtained in 'pure' conduction band impurity alloys. In realistic alloy systems, competition exists between the above two kinds of disorder, which may give rise to a transition in the residual MR from positive to negative with increase in the Kondo-hole concentration.

1. Introduction

A very important problem in the research of normal heavy-fermion (HF) systems is the 'coherence'. It is found that, at a relatively high temperature $T > T^*$ (T^* is the characteristic temperature of HF systems), there is a logarithmically increasing component of electrical resistivity with decreasing temperature, and the magnetic susceptibility follows the Curie–Weiss law. This means that the f ions in HF compounds behave as independent Kondo ions in the high-temperature region. However, in the low-temperature region when $T < T^*$, the resistivity decreases dramatically after reaching a peak, and the magnetic susceptibility becomes of Pauli type. It is said that, at this time, the HF compounds have coherent states because of the correlation between f ions.

In order to obtain more information about the coherent states, much attention has been focused on Kondo-hole alloys such as $Ce_{1-x}La_xCu_6$ and $Ce_{1-x}La_xAl_3$, in which the f ions are substituted by non-f ions. From the experimentally revealed temperature-dependent resistivity of this alloy system, it is believed that the coherence is set up gradually with increase in the f-ion concentration [1, 2]. Another interesting and puzzling property of Kondo-hole alloys is the magnetoresistivity (MR) of this system. In Kondo lattices such as $CeCu_6$, a positive residual MR has been observed [3–6], whereas for Kondo-hole alloys, when x is not close to unity, the MR is negative at any temperature. Obviously, the MR is strongly dependent on the f-ion concentration, and study of the MR is of great significance to the understanding of the nature of the HF alloys.

In this paper, we present our theoretical investigation of the HF alloys with both non-f impurities (Kondo holes) and conduction band impurities (CB impurities). The slave-boson technique is used to deal with the strong f–f correlation in HF systems, and the influences on the residual MR for the two kinds of impurity are studied in the single-site coherent-potential approximation (CPA). The rest of this paper is organized as follows. In section 2, the slave-boson mean-field (SBMF) Hamiltonian of the HF alloys is presented. In section 3, the effective-medium and the mean-field parameters are determined self-consistently. In section 4, we calculate the residual MR of the HF alloys, and the different effects on residual

MR of the two kinds of impurity are obtained. In section 5, we present the conclusion and some discussion.

2. The Hamiltonian of HF alloys

The $U = \infty$ periodic Anderson model (PAM) is considered to be a fundamental description of the Kondo lattice [7, 8]. In order to obtain a metallic ground state in the half-filled condition, we assume that there are two conduction bands mixing with f electrons. Using the slave-boson technique, the two-conduction-band PAM can be written as

$$H_0 = \sum_{i=1,2} \sum_{k\tau} \varepsilon_{ik} d_{ik\tau}^+ d_{ik\tau} + \sum_{l\tau} E_0 f_{l\tau}^+ f_{l\tau} + V \sum_i \sum_{l\tau} (d_{il\tau}^+ f_{l\tau} b_l^+ + f_{l\tau}^+ d_{il\tau} b_l) \tag{1}$$

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

$$\sum_\tau f_{l\tau}^+ f_{l\tau} + b_l^+ b_l = 1 \tag{2}$$

where $\tau = \pm 1$ is the spin index and $d_{ik\tau}(f_{l\tau})$ is the annihilation operator of the ith conduction band (localized) electron in the Bloch (Wannier) representation. We assume that the two conduction bands have the same dispersion ε_k, and that

$$\varepsilon_{1,2k} = \varepsilon_k \pm \varepsilon_0. \tag{3}$$

For simplicity, the density of states (DOS) of the unperturbed conduction electrons is assumed to be a constant with a band width $2D$.

The effect of the applied magnetic field is to add a Zeeman term in both the conduction and the f-electron energies:

$$\varepsilon_{ik\tau} = \varepsilon_{ik} + \tau h \tag{4}$$

$$E_{0\tau} = E_0 + \tau h \tag{5}$$

where h is the reduced magnetic field: $h = g\mu_B B$. Here we assume that the conduction electrons and the f electrons have the same Landé factor g.

In the mean-field approximation, both b and b^+ can be replaced by a c-number r, and a Lagrange multiplier λ is introduced to ensure satisfaction of the constraint (2). Then the effective Hamiltonian can be written as

$$H_0' = \sum_{ik\tau} \varepsilon_{ik\tau} d_{ik\tau}^+ d_{ik\tau} + \sum_{l\tau} E_{f\tau} f_{l\tau}^+ f_{l\tau} + rV \sum_{il} \sum_\tau (d_{il\tau}^+ f_{l\tau} + f_{l\tau}^+ d_{il\tau}) \tag{6}$$

where

$$E_{f\tau} = E_{0\tau} + \lambda. \tag{7}$$

The mean-field parameters λ and r are determined by the minimum condition of the free energy, which can be expressed as

$$\sum_\tau \langle f_{l\tau}^+ f_{l\tau} \rangle + r^2 = 1 \tag{8}$$

$$2N\lambda r + V \sum_{il\tau} \langle f_{l\tau}^+ d_{il\tau} + d_{il\tau}^+ f_{l\tau} \rangle = 0. \tag{9}$$

Now let us discuss the effects of impurities. One kind of impurity is Kondo holes, which occur when the f (Ce-like) ions are substituted by non-f (La-like) ions. In order to ensure that there is no f-electron occupation on the Kondo hole, we should take the f-electron energy E_L to be infinite in the impurity site. There exists another kind of substitution which is caused by conduction band impurities, as in the alloy $CeCu_{6-x}Al_x$. The main effect of the CB impurities is to bring about a change in the cell volume of the impurity site, which then gives rise to a change in the conduction–f mixing strength. In an alloy in which both impurities exist, the SBMF Hamiltonian is

$$\mathbf{H} = \sum_{k\tau}(d^+_{1k\tau} d^+_{2k\tau} f^+_{k\tau})\mathbf{E}_{0\tau}(k)\begin{bmatrix} d_{1k\tau} \\ d_{2k\tau} \\ f_{k\tau}\end{bmatrix} + \sum_{l\tau}(d^+_{1l\tau} d^+_{2l\tau} f^+_{l\tau})\mathbf{V}_l\begin{bmatrix} d_{1l\tau} \\ d_{2l\tau} \\ f_{l\tau}\end{bmatrix} \tag{10}$$

with

$$\mathbf{E}_{0\tau}(k) = \begin{bmatrix} \varepsilon_{1\tau} & 0 & 0 \\ 0 & \varepsilon_{2\tau} & 0 \\ 0 & 0 & E_{f\tau}\end{bmatrix} \tag{11}$$

and

$$\mathbf{V}_l = \begin{cases} \mathbf{V}_0 = \begin{bmatrix} 0 & 0 & rV \\ 0 & 0 & rV \\ rV & rV & 0\end{bmatrix} & \text{for a site with an f ion} \\ \mathbf{V}_K = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \varepsilon_L\end{bmatrix} & \begin{array}{l}\text{for a site with a Kondo hole,} \\ \text{and } \varepsilon_L = E_L - E_{f\tau} \text{ is taken} \\ \text{to be infinite at the end of the calculation}\end{array} \\ \mathbf{V}_C = \begin{bmatrix} 0 & 0 & rV' \\ 0 & 0 & rV' \\ rV' & rV' & 0\end{bmatrix} & \begin{array}{l}\text{for a site with a CB impurity,} \\ \text{where the conduction–f mixing strength} \\ \text{changes from } V \text{ to } V'\end{array}\end{cases} \tag{12}$$

where $\mathbf{V}_l$ is a disorder potential due to Kondo holes and CB impurities, which are distributed randomly on the lattice sites of PAM. Therefore, the Hamiltonian (10) cannot be diagonalized by the standard procedure. In order to solve this disorder system self-consistently, we shall adopt the single-site CPA.

3. The effective medium

In the framework of CPA, the HF alloy systems in the magnetic field can be described by an effective Hamiltonian $\tilde{\mathbf{H}}$ [9, 10]

$$\tilde{\mathbf{H}} = \sum_{k\tau}(d^+_{1k\tau} d^+_{2k\tau} f^+_{k\tau})[\mathbf{E}_{0\tau}(k) + \Sigma^\tau]\begin{bmatrix} d_{1k\tau} \\ d_{2k\tau} \\ f_{k\tau}\end{bmatrix}. \tag{13}$$

Although the Hamiltonian (13) is bilinear in the electron creation and annihilation operators, it is still impossible to obtain the quasi-particle spectrum by the simple diagonalization of equation (13) because the coherent potential Σ is energy dependent, and it must be calculated self-consistently from the following equation [9]:

$$(1 - C_I - C_{KH})\mathbf{t}^\tau_0 + C_I\mathbf{t}^\tau_c + C_{KH}\mathbf{t}^\tau_K = 0 \tag{14}$$

where $C_{\rm I}$ and $C_{\rm KH}$ are the concentrations of CB impurities and Kondo holes, respectively, and $\mathbf{t}_i^\tau$ is the scattering **t**-matrix:

$$\mathbf{t}^\tau_{i(i=0,c,K)} = (V_i - \Sigma^\tau)[1 - \mathbf{F}^\tau(V_i - \Sigma^\tau)]^{-1} \tag{15}$$

with

$$\mathbf{F}^\tau = \begin{bmatrix} F^\tau_{11} & F^\tau_{12} & F^\tau_{1f} \\ F^\tau_{21} & F^\tau_{22} & F^\tau_{2f} \\ F^\tau_{f1} & F^\tau_{f2} & F^\tau_{ff} \end{bmatrix} \qquad F^\tau_{ij} = \frac{1}{N}\sum_k G^\tau_{ij}(k,\omega) \tag{16}$$

where $G^\tau_{ij}(k,\omega)$ is the matrix element of the Green function corresponding to the effective Hamiltonian $\tilde{H}$:

$$\mathbf{G}^\tau(k,\omega) = (\omega - \Sigma^\tau - \mathbf{E}_{0\tau})^{-1}. \tag{17}$$

The mean-field parameters r and λ of the alloy systems are also determined by the minimum condition of the free energy. In the effective-medium potential Σ, the systems are site invariant; therefore, equations (8) and (9) are rewritten as

$$\frac{1}{N(1-C_{\rm KH})}\sum_{k\tau}\langle f^+_{k\tau} f_{k\tau}\rangle + r^2 = 1 \tag{18}$$

$$2r\lambda + \frac{1}{(1-C_{\rm KH})N}[V(1-C_{\rm KH}) + \Delta V C_{\rm I}]\sum_{ik\tau}\langle d^+_{ik\tau} f_{k\tau} + f^+_{k\tau} d_{ik\tau}\rangle = 0 \tag{19}$$

where N is the number of sites, and $\Delta V \equiv V' - V$. The chemical potential μ is determined by the total number of electrons:

$$\frac{1}{N}\sum_{ik\tau}(\langle f^+_{k\tau} f_{k\tau}\rangle + \langle d^+_{ik\tau} d_{ik\tau}\rangle) = 2 + (1 - C_{\rm KH}) \tag{20}$$

where we have ignored the influence on the electron number due to the CB impurities.

4. Residual MR of HF alloys

First, let us consider a special case of HF alloys in which only Kondo holes exist. It has been proved that the effective medium has the simple form as in [11, 12]:

$$\Sigma^\tau = \begin{bmatrix} 0 & 0 & rV \\ 0 & 0 & rV \\ rV & rV & \Sigma^\tau_{ff} \end{bmatrix} \tag{21}$$

where Σ^τ_{ff} can be calculated from

$$\Sigma^\tau_{ff} F^\tau_{ff} = -C_{\rm KH}. \tag{22}$$

In the single-site CPA, the conductivity at temperature T in the presence of magnetic field can be expressed as [13]

$$\sigma(T) = \frac{e^2}{3\pi\Omega m^2}\int_{-\infty}^{\infty} d\omega \left(-\frac{\partial f}{\partial \omega}\right)\sum_{k\tau} v_k^2 [\![\{\mathrm{Im}[G^\tau_{11}(k,\omega+i0^+)]\}^2 + \{\mathrm{Im}[G^\tau_{22}(k,\omega+i0^+)]\}^2]\!] \tag{23}$$

where $f(\omega)$ is the Fermi distribution function. Setting $T = 0$ in equation (23), we can easily obtain the residual resistivity of the system as

$$\sigma_0 = \frac{e^2}{3\pi\Omega m^2} \sum_{k\tau} v_k^2(\mu) [\![\{\mathrm{Im}[G_{11}^{\tau}(k, \mu + \mathrm{i}0^+)]\}^2 + \{\mathrm{Im}[G_{22}^{\tau}(k, \mu + \mathrm{i}0^+)]\}^2]\!] . \tag{24}$$

Figure 1 shows the calculated residual resistivity of Kondo-hole alloys in zero and non-zero magnetic field. It is found that the calculated residual resistivity deviates from the Nordheim law, and it is always suppressed by the applied magnetic field for any impurity concentration. Therefore, we have negative residual MR for Kondo holes.

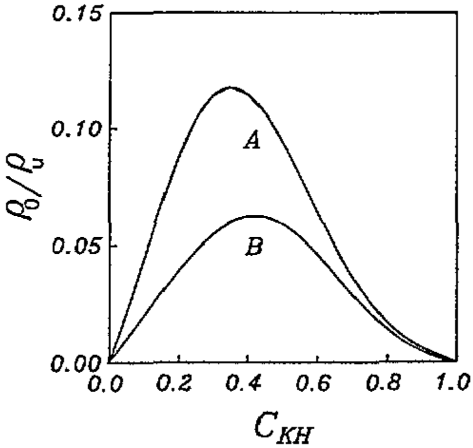

Figure 1. The residual resistivity of Kondo-hole alloys: curve A, $h = 0$; curve B, $h = 5 \times 10^{-4} D$, $\rho_u \equiv 3\pi\Omega m^2/e^2$. C_{KH} is the concentration of Kondo holes.

Now, let us discuss the magnetotransport property of the alloy with only CB impurities. In the absence of Kondo holes when $C_{\mathrm{KH}} = 0$, Σ has the form

$$\Sigma^{\tau} = \begin{bmatrix} \Sigma_1^{\tau} & \Sigma_1^{\tau} & \Sigma_2^{\tau} \\ \Sigma_1^{\tau} & \Sigma_1^{\tau} & \Sigma_2^{\tau} \\ \Sigma_2^{\tau} & \Sigma_2^{\tau} & \Sigma_3^{\tau} \end{bmatrix} . \tag{25}$$

The CPA equation is

$$(1 - C_{\mathrm{I}})\mathbf{t}_0^{\tau} + C_{\mathrm{I}}\mathbf{t}_{\mathrm{c}}^{\tau} = 0 \tag{26}$$

where $\mathbf{t}_0^{\tau}$ and $\mathbf{t}_{\mathrm{c}}^{\tau}$ satisfy equations (15)–(17).

In the dilute limit when $C_{\mathrm{I}} \ll 1$, equation (26) can be simplified as

$$\Sigma^{\tau}(\omega) = C_{\mathrm{I}}\Delta\mathbf{H}[1 - F_0^{\tau}(\omega)\Delta\mathbf{H}]^{-1} \tag{27}$$

where

$$\Delta\mathbf{H} = \begin{bmatrix} 0 & 0 & r\Delta V \\ 0 & 0 & r\Delta V \\ r\Delta V & r\Delta V & 0 \end{bmatrix} \tag{28}$$

and

$$F_0^{\tau}(\omega) = \frac{1}{N}\sum_k(\omega - \mathbf{E}_{0\tau})^{-1}. \tag{29}$$

Since we have $\Sigma^{\tau}(\omega) \propto C_I$ from equation (27), it is easy to find that, when $C_I \ll 1$, the residual resistivities of the system are proportional to C_I (the concentration of CB impurities) in both zero and non-zero magnetic fields, as we have pointed out in [14].

By the self-consistent calculation of equation (26), we may also obtain the residual MR of the CB-impurity alloy. The numerical results of the residual resistivity in zero and non-zero magnetic fields are sketched in figure 2(*a*). Obviously, the residual resistivity of CB impurities is very small compared with that of Kondo holes. However, the magnetic field enhances the residual resistivity dramatically, resulting in a large positive residual MR for CB impurities. In figure 2(*b*), we also give the residual resistivities in zero and non-zero magnetic fields in the region of $0 \leqslant C_I \leqslant 1\%$. It is easily found that they are all linear functions of C_I in accordance with the above prediction in the dilute limit.

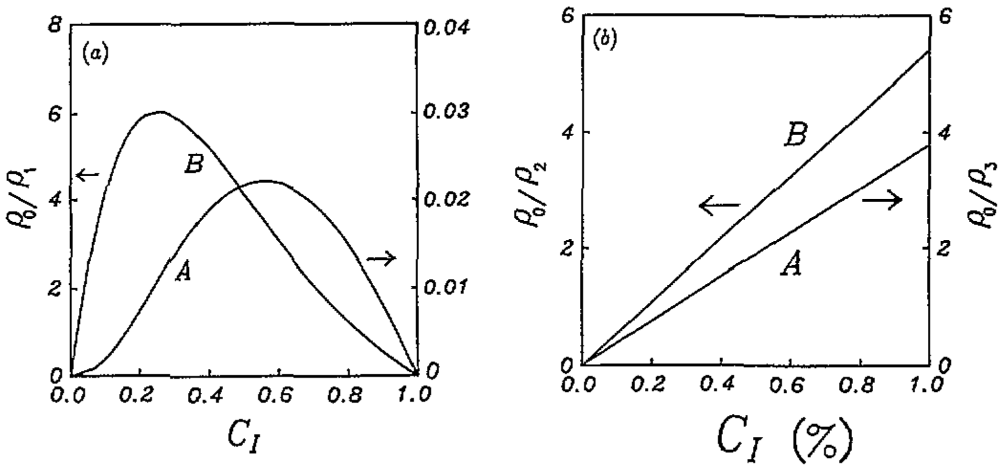

Figure 2. (*a*) The residual resistivity of CB-impurity alloys: curve A, $h = 0$; curve B, $h = 5 \times 10^{-4}D$, $\Delta V = 0.1D$, $\rho_1 \equiv 3 \times 10^{-4}\pi\Omega m^2/e^2$. C_I is the concentration of CB impurities. (*b*) The residual resistivity of CB-impurity alloys in the region $0 \leqslant C_I \leqslant 1\%$: curve A, $h = 0$; curve B, $h = 5 \times 10^{-4}D$, $\rho_2 \equiv 3 \times 10^{-5}\pi\Omega m^2/e^2$, $\rho_3 \equiv 3 \times 10^{-9}\pi\Omega m^2/e^2$.

In an alloy with the above two kinds of impurity, we have to calculate the full CPA equations but, in the dilute case when both $C_I \ll 1$ and $C_{KH} \ll 1$, the correlation between these two sorts of disorder can be neglected. In this condition, we can use the Matthiessen rule and obtain

$$\rho_0(h) = \rho_{0c}(h) + \rho_{0K}(h) \tag{30}$$

where $\rho_{0c}(h)$ and $\rho_{0K}(h)$ are proportional to C_I and C_{KH}, respectively. At this time, there is competition between the Kondo-hole-induced negative MR and the CB-impurity-induced positive MR, and there must be a critical value C_{KH}^{cr} of C_{KH} at which the residual MR changes sign with definite magnetic field h and C_I.

In a realistic material such as $Ce_xLa_{1-x}Cu_6$, besides the Kondo holes induced by the substitution of La, there must be some randomly distributed impurities and defects. They may produce a fluctuation in the conduction–f mixing strength just as the CB impurities do. Therefore, competition between positive and negative residual MRs occur, and the critical C_{KH}^{cr} concentration of Kondo holes must be magnetic field and sample dependent. For example, in the alloy $Ce_{1-x}La_xCu_6$ with 5% CB impurities, if we assume that the variation in conduction–f mixing strength induced by CB impurities is $\Delta V = 0.1D$, within a magnetic field $h = 3.5 \times 10^{-4}D$, the critical concentration of Kondo holes with which the residual MR of the alloy changes sign is $x_c \equiv C_{KH}^{cr} \simeq 0.01\%$. If we take $\Delta V = -0.1D$ and $h = 2 \times 10^{-4}D$, we have $x_c \equiv C_{KH}^{cr} \simeq 0.15\%$. For the realistic material in which ΔV and C_I are relatively small, the Kondo holes produce a larger negative MR than the positive MR produced by CB impurities. In this condition, C_{KH}^{cr} should have a small value.

5. Conclusion and discussion

In this paper, we have carried out some theoretical research on the residual MR of HF alloys. We have first provided a SBMF model of HF alloys with both Kondo holes and CB impurities. Then the effects of impurities have been represented by the effective medium in the single-site CPA. Including the magnetic field dependence of the SBMF parameters, the residual MRs of HF alloys with different impurities have been calculated. Our results show that only a negative residual MR can be obtained in 'pure' Kondo-hole alloys and only a positive residual MR can be obtained in 'pure' CB-impurity alloys. In a realistic alloy system, there must be competition between different kinds of disorder, which will give rise to transition of the residual MR from positive to negative when the Kondo-hole concentration increases.

In our calculation, we have assumed a constant variation in conduction–f mixing strength and have also neglected multiple scattering among impurities. We believe that these approximations do not qualitatively modify the results. At finite temperatures, the thermal fluctuations contribute a T^2-term to the resistivity in HF alloys [15]. The extension of our study on MR to finite temperatures will be very interesting. However, it is rather difficult to evaluate the MR coefficient of the T^2-term for the alloy system. This work is being investigated, and the results will be published elsewhere.

Acknowledgments

The authors are grateful to Dr W Xu for helpful discussions. This work was supported by the National Natural Science Foundation of China.

References

[1] Sumiyama A, Oda Y, Nagano H, Onuki Y, Shimutani K and Komatsubara T 1986 *J. Phys. Soc. Japan* **55** 1294

[2] Grewe N and Steglich F 1991 *Handbook of the Physics and Chemistry of Rare Earths* vol 14 (New York: Elsevier) p 343

[3] Sumiyama A, Oda Y, Nagano H, Onuki Y and Komatsubara T 1985 *J. Phys. Soc. Japan* **54** 4470

[4] Amato A, Jaccard D, Flouquet J, Lapierre F, Tholence J L, Fisher R A, Lacy S E, Olsen J A and Phillips N E 1987 *J. Low. Temp. Phys.* **68** 371

[5] Coleridge P T 1987 *J. Phys. F: Met. Phys.* **17** L79

[6] Mignot J M, Ponchet A, Haen P, Lapierre F and Flouquet J 1989 *Phys. Rev.* B **40** 10917

[7] Auerbach A and Levin K 1986 *Phys. Rev. Lett.* **57** 877; 1986 *Phys. Rev.* B **34** 3524
[8] Mills A J and Lee P A 1987 *Phys. Rev.* B **35** 3394
[9] Yenezawa T 1982 *The Structure and Properties of Matter* ed T Matsubara (Berlin: Springer) ch 11
[10] Wiethege W, Costi T and Entel P 1985 *Z. Phys.* B **60** 189
[11] Li Z Z, Qiu Y and Xu W 1988 *Phys. Lett.* **131A** 466
[12] Xu W and Li Z Z 1988 *J. Phys. C: Solid State Phys.* **21** 598
[13] Velicky B 1964 *Phys. Rev.* **184** 614
[14] Chen C, Li Z Z and Xu W 1993 *J. Phys.: Condens. Matter* **5** 95
[15] Xu W and Li Z Z 1990 *J. Phys.: Condens. Matter* **2** 109