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Resistivity in the extended slave-boson mean field theory of the Anderson alloy system

Kikuo Harigaya
Department of Physics, University of Tokyo, Bunkyo-ku, Tokyo 113, Japan

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Abstract. Resistivity in the Anderson alloy system is calculated using the extended slave-boson mean field theory developed by Xu and Li. We find that the value of the peak of resistivity as a function of concentration of magnetic ions is very close to that of the experimentally observed Nordheim law. As the condition of the coherent potential approximation (CPA) violates the dual symmetry, resistivity is not symmetric with respect to the point of half concentration. The concentration of the peak is close to that of the previous Yoshimori–Kasai result. The fact that this feature may be intrinsic to the formalism of the single-site CPA is discussed.

1. Introduction

It is known that the alloy system of magnetic and non-magnetic ions shows a rich variation in low temperature electronic properties [1]. With an increasing concentration of magnetic ions, the system changes from the dilute Kondo system, through the dense Kondo system, and finally to the Kondo lattice. This change is reflected in various physical quantities. For the transport, the Nordheim law has been observed in the residual resistivity ρ at $T = 0$ K, for instance in $Ce_xLa_{1-x}Cu_2Si_2$ [2] and $Ce_xLa_{1-x}Cu_6$ [3]. It varies as $\rho = \rho_0 x(1-x)$, where ρ_0 is the single-impurity resistivity.

There are a few examples of theoretical calculations of the residual resistivity, for instance by Yoshimori and Kasai [4]. They extended the finite-U single-impurity theory to the alloy system making use of the single-site version of the coherent potential approximation (CPA) [5]. However, this approximation has been applied by many authors to calculating the density of states of the Anderson alloy system, but different approximation schemes for strong correlation among electrons have been used. For example, the one-dimensional Anderson alloy, with a finite strength for the Coulomb repulsion, is analysed [6], and the slave-boson mean field theory is extended to the alloy system [7].

In this paper, we calculate residual resistivity making use of the extended slave-boson mean field theory of Xu and Li [7]. Mean field parameters and the coherent potential are computed self-consistently as functions of the concentration of magnetic ions. Electric resistivity is calculated at $T = 0$ K. We find that the value of the peak of resistivity is very close to that of the Nordheim law. As the condition of the CPA violates the dual symmetry, resistivity is not symmetric with respect to the point of half concentration. Comparison with the Yoshimori–Kasai result is made and possible directions for the revision of the theory are discussed.

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In the next section, the application of the single-site CPA to the mean field theory of the Anderson alloy is reviewed and the formula for resistivity is given. In section 3, we present numerical results and discuss the findings.

2. Formalism

The slave-boson technique [8] for the infinite-U Anderson impurity and lattice models can also be applied to the Anderson alloy model. We consider, in particular, the alloy system where Ce and La are located at the magnetic and non-magnetic sites, respectively. The Hamiltonian is

$$\mathcal{H} = \sum_{i\sigma} [\xi_i(-E_f) + (1-\xi_i)E_f^{La}] f_{i\sigma}^\dagger f_{i\sigma} + \sum_{k\sigma} \varepsilon_k c_{k\sigma}^\dagger c_{k\sigma} + V \sum_{i\sigma} \xi_i (b_i^\dagger c_{i\sigma}^\dagger f_{i\sigma} + f_{i\sigma}^\dagger c_{i\sigma} b_i) + \sum_i \xi_i \lambda_i \left(\sum_\sigma f_{i\sigma}^\dagger f_{i\sigma} + b_i^\dagger b_i - 1 \right) \tag{2.1}$$

where ξ_i is a random variable which is defined as

$$\xi_i = \begin{cases} 1 & \text{if the atom of the } i\text{th site is Ce} \\ 0 & \text{if it is La.} \end{cases} \tag{2.2}$$

The variable $f_{i\sigma}$ annihilates an f electron with spin σ at the ith site. The energy of an f electron at the Ce site is $-E_f$, where the relation $E_f > 0$ is assumed. In the course of the calculation, the limit $E_f^{La} \to \infty$ is taken in order to ensure that there are no f electrons at the La site. The quantity $c_{k\sigma}$ is an annihilation operator of the conduction electron with the momentum $\boldsymbol{k}$ and spin σ. It is connected to $c_{i\sigma}$ via the relation

$$c_{i\sigma} = N^{-1/2} \sum_{\boldsymbol{k}} \exp(i\boldsymbol{k} \cdot \boldsymbol{R}_i) c_{k\sigma}.$$

Constant density of states per site is assumed for the conduction electrons; the value is $1/2D$ for $-D < \varepsilon_k < D$, and zero, otherwise. The operator b_i annihilates the slave boson that is introduced in order to exclude double occupancy of f electrons at the Ce site. The condition of infinite strength of the repulsive force is represented by the last term of (2.1); the constraint

$$\sum_\sigma f_{i\sigma}^\dagger f_{i\sigma} + b_i^\dagger b_i = 1 \tag{2.3}$$

is added with the Lagrange multiplier λ_i.

The CPA [5] has been applied successfully [7] to calculate the electronic density of states of the Anderson alloy system with the *ansatz* of the mean field approximation: $\langle b_i \rangle = r$ and $\lambda_i = \lambda$ for all i. We apply the same formalism to calculate the resistivity. The only difference is in the number of the conduction bands; in [7], they assumed two conduction bands.

In the mean field theory, equation (2.1) is rewritten as

$$\mathcal{H}_{MF} = \sum_{i\sigma} \left[\xi_i \Psi_{i\sigma}^\dagger \begin{pmatrix} \tilde{E}_f & rV \\ rV & 0 \end{pmatrix} \Psi_{i\sigma} + (1-\xi_i) \Psi_{i\sigma}^\dagger \begin{pmatrix} E_f^{La} & 0 \\ 0 & 0 \end{pmatrix} \Psi_{i\sigma} \right] + \sum_{k\sigma} \varepsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \lambda(r^2 - 1) \sum_i \xi_i \tag{2.4}$$

where the effective f level is defined as $\tilde{E}_f = -E_f + \lambda$, and $\Psi_{i\sigma}$ is a two-component operator:

$$\Psi_{i\sigma} = \begin{pmatrix} f_{i\sigma} \\ c_{i\sigma} \end{pmatrix}. \tag{2.5}$$

We define a matrix propagator of the uniform system as

$$\mathbf{G}_0(\tau, \boldsymbol{k}) = -\langle T_\tau \Psi_{k\sigma}(\tau) \Psi_{k\sigma}^\dagger(0) \rangle. \tag{2.6}$$

Its Fourier transform with respect to the imaginary time τ is

$$\mathbf{G}_0^{-1}(\mathrm{i}\omega_n, \boldsymbol{k}) = \begin{pmatrix} \mathrm{i}\omega_n - \tilde{E}_f & 0 \\ 0 & \mathrm{i}\omega_n - \varepsilon_k \end{pmatrix} \tag{2.7}$$

where $\omega_n = (2n+1)\pi T$ is the odd Matsubara frequency. When the potential fluctuations at Ce and La sites are expressed by

$$\delta \mathbf{V}_{\mathrm{Ce}} = \begin{pmatrix} 0 & rV \\ rV & 0 \end{pmatrix} \tag{2.8a}$$

and

$$\delta \mathbf{V}_{\mathrm{La}} = \begin{pmatrix} E_f^{\mathrm{La}} - \tilde{E}_f & 0 \\ 0 & 0 \end{pmatrix} \tag{2.8b}$$

we write the condition of the single-site CPA as

$$c(\delta \mathbf{V}_{\mathrm{Ce}} - \boldsymbol{\Sigma})[\mathbf{1} - \bar{\mathbf{g}}(\delta \mathbf{V}_{\mathrm{Ce}} - \boldsymbol{\Sigma})]^{-1} + (1-c)(\delta \mathbf{V}_{\mathrm{La}} - \boldsymbol{\Sigma})[\mathbf{1} - \bar{\mathbf{g}}(\delta \mathbf{V}_{\mathrm{La}} - \boldsymbol{\Sigma})]^{-1} = 0 \tag{2.9}$$

where c is the Ce concentration, the coherent potential $\boldsymbol{\Sigma}$ is given in a 2×2 matrix, and $\bar{\mathbf{g}}$ is the single-site propagator:

$$\bar{\mathbf{g}} = N^{-1} \sum_{\boldsymbol{k}} \bar{\mathbf{G}}(\mathrm{i}\omega_n, \boldsymbol{k}).$$

Here, the effective medium propagator is given by $\bar{\mathbf{G}}(\mathrm{i}\omega_n, \boldsymbol{k}) = (\mathbf{G}_0^{-1}(\mathrm{i}\omega_n, \boldsymbol{k}) - \boldsymbol{\Sigma}(\mathrm{i}\omega_n))^{-1}$. After the limit $E_f^{\mathrm{La}} \to \infty$ is taken in (2.9), we obtain

$$\boldsymbol{\Sigma} = \begin{pmatrix} \Sigma_f & rV \\ rV & 0 \end{pmatrix}. \tag{2.10}$$

Then, we can write explicitly

$$\bar{\mathbf{G}}(\mathrm{i}\omega_n, \boldsymbol{k}) \equiv \begin{pmatrix} \bar{G}_f(\mathrm{i}\omega_n, \boldsymbol{k}) & \bar{A}(\mathrm{i}\omega_n, \boldsymbol{k}) \\ \bar{A}(\mathrm{i}\omega_n, \boldsymbol{k}) & \bar{G}_c(\mathrm{i}\omega_n, \boldsymbol{k}) \end{pmatrix}$$

$$= \frac{1}{(\mathrm{i}\omega_n - \tilde{E}_f - \Sigma_f)(\mathrm{i}\omega_n - \varepsilon_k) - r^2 V^2} \begin{pmatrix} i\omega_n - \varepsilon_k & rV \\ rV & \mathrm{i}\omega_n - \tilde{E}_f - \Sigma_f \end{pmatrix} \tag{2.11}$$

where $\Sigma_f(\mathrm{i}\omega_n)$ is determined by the reduced condition

$$\bar{g}_f(\mathrm{i}\omega_n)\Sigma_f(\mathrm{i}\omega_n) = c - 1 \tag{2.12a}$$

with

$$\bar{g}_{\mathrm{f}}(\mathrm{i}\omega_n) = \frac{1}{N}\sum_{k} \bar{G}_{\mathrm{f}}(\mathrm{i}\omega_n, \boldsymbol{k}) = \frac{1}{\mathrm{i}\omega_n - \tilde{E}_{\mathrm{f}} - \Sigma_{\mathrm{f}}}\left[1 - \frac{r^2V^2}{2D(\mathrm{i}\omega_n - \tilde{E}_{\mathrm{f}} - \Sigma_{\mathrm{f}})}\right.$$
$$\left.\times \mathrm{Log}\left(\frac{(\mathrm{i}\omega_n - D)(\mathrm{i}\omega_n - \tilde{E}_{\mathrm{f}} - \Sigma_{\mathrm{f}}) - r^2V^2}{(\mathrm{i}\omega_n + D)(\mathrm{i}\omega_n - \tilde{E}_{\mathrm{f}} - \Sigma_{\mathrm{f}}) - r^2V^2}\right)\right] \tag{2.12b}$$

where Log means the principal value of the logarithm.

The parameters r and λ are determined by two self-consistency equations. One is the condition of free energy minimum with respect to r

$$\frac{2V}{c}\frac{T}{N}\sum_{nk} \bar{A}(\mathrm{i}\omega_n, \boldsymbol{k}) + r\lambda = 0 \tag{2.13}$$

and the other is the constraint (2.3)

$$\frac{2}{c}\frac{T}{N}\sum_{nk} \bar{G}_{\mathrm{f}}(i\omega_n, \boldsymbol{k}) + r^2 = 1. \tag{2.14}$$

As shown in [7], the fundamental set of equations (2.12*a*), (2.13), and (2.14) for determining Σ_{f}, r, and λ, smoothly and naturally interpolates two mean field theories for the Anderson impurity and the Anderson lattice.

Electric conductivity is calculated by the Kubo formula for the isotropic system

$$\sigma(\omega) = e^2 \int \frac{\mathrm{d}\varepsilon}{2\pi}\frac{f(\varepsilon - \omega) - f(\varepsilon)}{\omega}\frac{1}{N}\sum_{k\sigma} \tfrac{1}{3}v^2(\boldsymbol{k})\,\mathrm{Tr}\,(\bar{\mathbf{G}}^{\mathrm{R}}(\varepsilon, \boldsymbol{k})\bar{\mathbf{G}}^{\mathrm{A}}(\varepsilon - \omega, \boldsymbol{k})) \tag{2.15}$$

where e is the charge on an electron, $f(x) = 1/(\exp(x/T) + 1)$, $\bar{\mathbf{G}}^{\mathrm{R}}(\varepsilon, \boldsymbol{k}) = \bar{\mathbf{G}}(\varepsilon + \mathrm{i}\delta, \boldsymbol{k})$, and $\bar{\mathbf{G}}^{\mathrm{A}}(\varepsilon, \boldsymbol{k}) = \bar{\mathbf{G}}(\varepsilon - \mathrm{i}\delta, \boldsymbol{k})$. It is not necessary to include the vertex correction in (2.15), because it is zero in the single-site CPA [5]. At $T = 0$, the static conductivity is given by

$$\sigma(0) = \frac{e^2}{3\pi}\frac{1}{N}\sum_{k} v^2(\boldsymbol{k})\,\mathrm{Tr}(\bar{\mathbf{G}}^{\mathrm{R}}(0, \boldsymbol{k})\bar{\mathbf{G}}^{\mathrm{A}}(0, \boldsymbol{k})). \tag{2.16}$$

Using the dispersion relation of the lower band

$$E_{-}(\boldsymbol{k}) = \tfrac{1}{2}[\varepsilon_k + \tilde{E}_{\mathrm{f}} + \mathrm{Re}\,\Sigma_{\mathrm{f}}(0) - \sqrt{(\varepsilon_k - \tilde{E}_{\mathrm{f}} - \mathrm{Re}\,\Sigma_{\mathrm{f}}(0))^2 + 4r^2V^2}] \tag{2.17}$$

and assuming $\varepsilon_k = \boldsymbol{k}^2/2m - D$, m being the mass of the conduction electrons, we obtain

$$v(\boldsymbol{k}) = \frac{\partial E_{-}(\boldsymbol{k})}{\partial|\boldsymbol{k}|} = \sqrt{\frac{\varepsilon_k + D}{2m}}\left(1 - \frac{\varepsilon_k - \tilde{E}_{\mathrm{f}} - \mathrm{Re}\,\Sigma_{\mathrm{f}}(0)}{[(\varepsilon_k - \tilde{E}_{\mathrm{f}} - \mathrm{Re}\,\Sigma_{\mathrm{f}}(0))^2 + 4r^2V^2]^{1/2}}\right). \tag{2.18}$$

Here, we have used the notation $\Sigma_{\mathrm{f}}(0) = \Sigma_{\mathrm{f}}(0 + \mathrm{i}\delta)$. Putting (2.11) and (2.18) into (2.16), we get

$$\sigma(0) = \frac{e^2}{6\pi m}\frac{1}{2D}\int_{-D}^{D} \mathrm{d}\varepsilon_k\,(\varepsilon_k + D)\left(1 - \frac{\varepsilon_k - \tilde{E}_{\mathrm{f}} - \mathrm{Re}\,\Sigma_{\mathrm{f}}(0)}{[(\varepsilon_k - \tilde{E}_{\mathrm{f}} - \mathrm{Re}\,\Sigma_{\mathrm{f}}(0))^2 + 4r^2V^2]^{1/2}}\right)^2$$
$$\times \frac{\varepsilon_k^2 + (\tilde{E}_{\mathrm{f}} + \mathrm{Re}\,\Sigma_{\mathrm{f}}(0))^2 + (\mathrm{Im}\,\Sigma_{\mathrm{f}}(0))^2 + 2r^2V^2}{[\varepsilon_k(\tilde{E}_{\mathrm{f}} + \mathrm{Re}\,\Sigma_{\mathrm{f}}(0)) - r^2V^2]^2 + [\varepsilon_k(\mathrm{Im}\,\Sigma_{\mathrm{f}}(0))]^2}. \tag{2.19}$$

Resistivity is given by the inverse of $\sigma(0)$: $\rho \equiv 1/\sigma(0)$.

With the help of forms of the dilute Ce concentration case

$$\bar{G}_f(i\omega_n, \boldsymbol{k}) = c\left(i\omega_n - \tilde{E}_f - \frac{r^2V^2}{N}\sum_p \frac{1}{i\omega_n - \varepsilon_p}\right)^{-1} \tag{2.20a}$$

$$\bar{G}_c(i\omega_n, \boldsymbol{k}) = \frac{1}{i\omega_n - \varepsilon_k} + cr^2V^2\left[(i\omega_n - \varepsilon_k)^2\left(i\omega_n - \tilde{E}_f - \frac{r^2V^2}{N}\sum_p \frac{1}{i\omega_n - \varepsilon_p}\right)\right]^{-1} \tag{2.20b}$$

and

$$\bar{A}(i\omega_n, \boldsymbol{k}) = crV\left[(i\omega_n - \varepsilon_k)\left(i\omega_n - \tilde{E}_f - \frac{r^2V^2}{N}\sum_p \frac{1}{i\omega_n - \varepsilon_p}\right)\right]^{-1} \tag{2.20c}$$

we calculate the single-impurity resistivity as

$$\rho_0 \equiv \lim_{c\to 0}\frac{1}{c}\rho = \frac{24mD}{e^2\pi}\frac{\tilde{\Delta}^2}{\tilde{E}_f^2 + \tilde{\Delta}^2} \tag{2.21}$$

where $\tilde{\Delta} = \pi r^2V^2/2D$ is the resonance width.

3. Numerical results and discussion

Results are mainly reported for parameters $D = 2 \times 10^4$ K, $V = 2500$ K, and $E_f = 3700$ K. Variation of E_f within 2000 K $\leq E_f \leq$ 15000 K does not change essential features of the solutions.

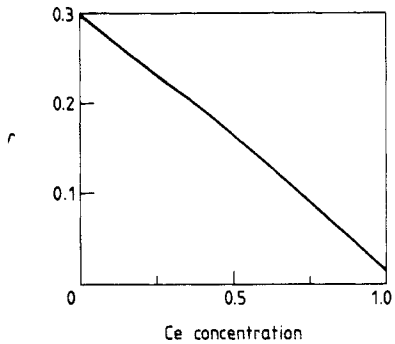

Figure 1. Ce concentration dependence of the mean field r.

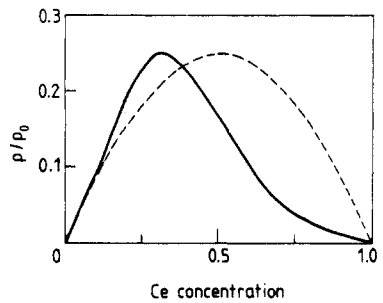

Figure 2. Electric resistivity as a function of the Ce concentration c. The full curve is for the current CPA result. The broken curve denotes the experimentally observed Nordheim law, $\rho = \rho_0 c(1-c)$, where ρ_0 is the single-impurity resistivity.

In figure 1, we present the concentration dependence of r. It varies almost linearly. Variation of r with respect to c seems to be stronger than that in [7], although similar magnitudes of parameters are assumed. This may be due to the difference in the number of degrees of freedom of the conduction electrons. As the effective f level $\tilde{E}_f$ has the magnitude of the Kondo temperature T_K at all the concentrations, λ is almost independent of c: $\lambda \simeq E_f$.

The electric resistivity ρ is calculated via (2.19) and is shown in figure 2 by the full curve. It is scaled by the single-impurity resistivity ρ_0. The experimentally observed Nordheim law, $\rho = \rho_0 c(1-c)$, is represented by the broken curve for comparison. A

positive gradient at $c = 0$ is common to both curves. With increasing c, the two curves deviate from each other. The full curve has a maximum at about $c = 0.3$. It decreases suddenly at $c > 0.3$. The two curves are separated to a remarkable degree at high concentrations.

We point out that the maximum value of ρ is close to that of the Nordheim law, $0.25\rho_0$. This may be because the single-site scattering process still plays a significant role in the alloy system. The development of mutual interference among magnetic ions with increasing concentration results in the crossover from the dilute Kondo system to the dense Kondo system. Finally, the Kondo lattice state is realised by developing complete coherence among magnetic ions.

We cannot show the Nordheim law starting from the CPA condition (2.12*a*). The reason for this is that it violates the dual symmetry [5] by including the approximation $E_f^{La} \to \infty$. The concentration, $c \simeq 0.3$, where ρ has a maximum, is very close to that of the Yoshimori–Kasai result [4]. This may be an intrinsic feature of the formalism of the single-site CPA, even though the approximation schemes for strong correlation among f electrons are different. It would be necessary to formulate the Anderson alloy system using the many-site CPA in order to describe the above-mentioned inter-site interference better and to overcome that defect of the single-site CPA. This problem needs further research.

We have assumed the site-independent mean field parameters r and λ. This is a valid approximation in the formalism of the single-site CPA; all lattice sites are equivalent and multiple scatterings among magnetic ions are neglected. Inclusion of site dependence might be necessary when the formalism is extended to the many-site CPA. Another method of treating the site dependence is numerical diagonalisation of a finite-size mean field Hamiltonian. Sample averaging enables us to check the validity of the CPA. The progress of future research in this direction will also be of interest.

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