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ELECTRICAL RESISTIVITY FOR THE NON-ORTHOGONAL ANDERSON MODEL

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The generalized non-orthogonal Anderson model is considered. Within the semiphenomenological simplifications the method of Green functions is applied to obtain the t-matrix for conduction electrons in terms of the self-energy of localized electrons. The localized electrons' self-energy is calculated in the second order with respect to the Coulomb potential. The temperature dependence of the low temperature electrical resistivity is discussed for different degrees of non-orthogonality.

1. *Introduction*

If one considers the problem of a localized impurity in a dilute alloy, two different approaches, one due to Anderson [1] and the other to Wolff [2], are commonly applied. In the Anderson Hamiltonian the impurity is represented by an extra orbital while in that of Wolff the impurity is considered as a localized potential i.e. as being constructed from the band states. These two models seem to be the limiting cases of the more general approach in which the impurity orbital is non-orthogonal to the band states, the overlap $\langle k|d\rangle$ of band and impurity states stands for the measure of non-orthogonality [3]. The local properties of the Anderson and Wolff models are equivalent if the details of the shape of the density of states are neglected [4]. The analogy breaks down when transport properties are considered [5].

The aim of the present paper is to obtain the results for electrical resistivity in terms of the above mentioned general model. Our recent work [6] shows how difficult it is to develop the thermodynamical theory in the general case. This causes that in order to obtain legible results, at least some semiphenomenological simplifications must necessarily be made.

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Our starting Hamiltonian is of the same form as in [6] i.e.

$$H = \sum_{k,\alpha} \varepsilon_k c^\dagger_{k\alpha} c_{k\alpha} + E \sum_{\alpha} a^\dagger_\alpha a_\alpha + \frac{V}{\sqrt{N}} \sum_{k,\alpha} c^\dagger_{k\alpha} a_\alpha + a^\dagger_\alpha c_{k\alpha} + U a^\dagger_\uparrow a_\uparrow a^\dagger_\downarrow a_\downarrow, \tag{1.1}$$

where

$$\{a_\alpha, c^\dagger_{k\alpha'}\} = \mu \frac{1}{\sqrt{N}} \delta_{\alpha\alpha'}, \quad \{a_\alpha, c_{k\alpha'}\} = 0 \tag{1.2}$$

$$\{a_\alpha, a^\dagger_{\alpha'}\} = \delta_{\alpha\alpha'}, \quad 0 \leqslant \mu \leqslant 1. \tag{1.3}$$

The notations are standard and we refer to [6] for details. For simplicity we assume that μ is k independent. We will perform the calculations in a way which assures that the number of impurity electrons $\langle a^\dagger_\alpha a_\alpha \rangle$ with spin α maintains itself at a constant value of 0.5. This should be interpreted such that in the limit $U \to \infty$ we are dealing with spin 1/2 which in general is composed from states which are not orthogonal to the band states.

2. *Calculations*

We want to calculate the impurity Green function

$$G_\alpha(\tau_1, \tau_2) = \frac{1}{i} \langle \hat{T}(a_\alpha(\tau_1) a^\dagger_\alpha(\tau_2)) \rangle, \tag{2.1}$$

$$G_\alpha(\tau_1, \tau_2) = \frac{i}{\beta} \sum_{z_\lambda} e^{-iz_\lambda(\tau_1 - \tau_2)} G_\alpha(z_\lambda), \quad z_\lambda = \frac{(2\lambda+1)\pi i}{\beta}, \tag{2.2}$$

where λ is an integer and the notations are the same as in our previous work [7]. The equation of motion for the analytic continuation of $G_\alpha(z_\lambda)$ can be written down as

$$G_\alpha(\omega) = G_{0\alpha}(\omega) + E G_{0\alpha}(\omega) G_\alpha(\omega) + U G_{0\alpha}(\omega) \Gamma_\alpha(\omega), \tag{2.3}$$

where

$$\Gamma_\alpha(\tau_1, \tau_2) = \frac{1}{i^2} \langle \hat{T}(a_\alpha(\tau_1) a_{-\alpha}(\tau_3) a^\dagger_{-\alpha}(\tau_3^\dagger) a^\dagger_\alpha(\tau_2)) \rangle_{\tau_3 = \tau_1}, \tag{2.4}$$

$$G_{0\alpha}(\omega) \equiv G_0(\omega) = [1 + \mu^2(\omega F - 1)] \{\omega - [2\mu V \omega + V^2(1-\mu^2)]F\}^{-1}, \tag{2.5}$$

$$F(\omega) = \frac{1}{N} \sum_k \frac{1}{\omega - \varepsilon_k}, \tag{2.6}$$

and $G_0(\omega)$ stands for the exact Green function for $E = U = 0$. We want to develop the perturbative calculus for $G(\omega)$ in a way similar to that exploited in [7]. This causes that some approximations should be made in (2.5). For the Lorentzian density of states

$$\varrho(\omega) = \frac{1}{\pi} \frac{D}{\omega^2 + D^2}, \tag{2.7}$$

it is reasonable to approximate (2.5) by

$$G_0(\omega) = \frac{1-\mu^2}{\omega+iV^2(1-\mu^2)D^{-1}} + \frac{\mu^2}{\omega+iD}$$

$$\equiv (1-\mu^2)G_{0\mathrm{A}}(\omega)+\mu^2 G_{0\mathrm{W}}(\omega). \tag{2.8}$$

The first term in (2.8) is the characteristic one for the Anderson model and the second for the Wolff model. Both terms contribute to the Green function with some weighting factors and it is apparent that $\langle a^\dagger_\alpha a_\alpha \rangle = 0.5$. Thus the feature that the impurity state is constructed from two types of electron states which contribute with normalized weighting factors is preserved. The resonant level half-width in the first term vanishes when $\mu \to 1$ and such a behaviour retains the general feature predicted by Rivier and Zitkova [3]. Certainly, for $\mu = 1$ or 0 we obtain the proper limiting forms of the Green function in both models.

We will consider the symmetric case $E = -\frac{1}{2}U$ which causes that the lowest order correction to the Green function is of the form [8, 7]

$$G^{(2)}(\tau_1, \tau_1') \equiv -(iU)^2 \int\limits_0^{-i\beta} G_0(\tau_1, \tau_2)G_0(\tau_2, \tau_3)G_0(\tau_3, \tau_2)G_0(\tau_2, \tau_3)G_0(\tau_3, \tau_1')d\tau_2 d\tau_3. \tag{2.9}$$

This enables us to obtain the second order proper self-energy. Staying in agreement with our simplification (2.8) we assume that the proper self-energy enters $G_0(\omega)$ such that

$$G(\omega) = (1-\mu^2)G_{0\mathrm{A}}(\omega-(1-\mu^2)\Sigma_\mu)+\mu^2 G_{0\mathrm{W}}(\omega-\mu^2\Sigma_\mu)$$

$$\equiv (1-\mu^2)G_{\mathrm{A}}(\omega)+\mu^2 G_{\mathrm{W}}(\omega), \tag{2.10}$$

which means that the terms of the type $(1-\mu^2)\mu^2 G_{0\mathrm{A}}\Sigma_\mu G_{0\mathrm{W}}$ are neglected. Thus the two types of electron states which contribute with weighting factors to the impurity state are renormalized in the same way by the self-energy which in turn depends on the values of the above mentioned weighting factors.

In order to derive the low temperature electrical resistivity we must find the t-matrix. On the basis of general results for the Anderson and Wolff models [5, 9] we can argue that we have two scattering factors being coupled to the band in different ways. In the considered symmetric case the coupling of the band part of impurity states is realized by the localized potential $\mu^2\Sigma_\mu$ and the coupling of the extra-orbital part by the hybridization potential $V\sqrt{1-\mu^2}$. Thus on the basis of such semiphenomenological argumentation we can write down the "effective" Hamiltonian which will be used to calculate the t-matrix

$$\tilde{H} = \sum_{k,\alpha} \varepsilon_k c^\dagger_{k\alpha} c_{k\alpha} + \Sigma_\mu\Big(\sum_\alpha d^\dagger_\alpha d_\alpha\Big) + \mu^2\Sigma_\mu\Big(\sum_\alpha c^\dagger_{0\alpha} c_{0\alpha}\Big)$$

$$+\frac{V\sqrt{1-\mu^2}}{\sqrt{N}} \sum_{k,\alpha} c^\dagger_{k\alpha} d_\alpha + d^\dagger_\alpha c_{k\alpha}, \tag{2.11}$$

$$\{d_\alpha, c^\dagger_{k\alpha'}\} = 0. \tag{2.12}$$

According to the usual definition [9] we find after simple calculations

$$t(\omega) = \mu^2 \Sigma_\mu G_c(\omega) F^{-1}(\omega) + V^2(1-\mu^2) G_d(\omega) \left[1-\mu^2 \Sigma_\mu F(\omega)\right]^{-1}, \tag{2.13}$$

where $G_c(\omega)$, $G_d(\omega)$ stand for the analytical continuations of the Fourier transforms of $i^{-1}\langle \hat{T}(c_{0\alpha}(\tau_1) c^\dagger_{0\alpha}(\tau_2))\rangle$ and $i^{-1}\langle \hat{T}(d_\alpha(\tau_1) d^\dagger_\alpha \tau_2))\rangle$ which in the symmetric case are spin independent. We should take into account that the two types of orbitals contribute to the scattering with the above mentioned weighting factors (the total number of localized electrons is 0.5 for each spin direction). Thus we make in (2.13) a replacement

$$G_c(\omega) \to \mu^2 G_{\mathrm{W}}(\omega), \qquad G_d(\omega) \to (1-\mu^2) G_{\mathrm{A}}(\omega), \tag{2.14}$$

which in some aspects restores the correlations which are lost in (2.11).

Σ_μ can be calculated in the second order with respect to U in the same way as previously [7] and we will not repeat the details here. The value of the imaginary part of the retarded t-matrix (t^{R}) at the Fermi surface gives direct information on the electrical resistivity at reasonable temperatures. Due to symmetry properties [7, 8] we find

$$-\operatorname{Im} t^{\mathrm{R}}(0) \cdot D^{-1} = \frac{\mu^4/D\, \Sigma_{i\mu}(\Sigma_{i\mu} - \Delta) + \tilde{\Delta}}{(1-\mu^2/D\, \Sigma_{i\mu})(\Delta - \Sigma_{i\mu})}, \tag{2.15}$$

$$\Delta = V^2 D^{-1}, \qquad \tilde{\Delta} = (1-\mu^2)\Delta, \tag{2.16}$$

where $\Sigma_{i\mu}$ stands for the imaginary part of the self-energy and is of the form

$$\begin{aligned} \Sigma_{i\mu} = {} & (1-\mu^2)^3 \Sigma_i(\tilde{\Delta}, \tilde{\Delta}, \tilde{\Delta}) + \mu^6 \Sigma_i(D, D, D) + (1-\mu^2)^2 \mu^2 [\Sigma_i(\tilde{\Delta}, \tilde{\Delta}, D) \\ & + \Sigma_i(D, \tilde{\Delta}, \tilde{\Delta}) + \Sigma_i(\tilde{\Delta}, D, \tilde{\Delta}) + \Sigma_i(D, D, \tilde{\Delta}) + \Sigma_i(\tilde{\Delta}, D, D) + \Sigma_i(D, \tilde{\Delta}, D)], \end{aligned} \tag{2.17}$$

$$\begin{aligned} \Sigma_i(a, b, c) = {} & \frac{0.5u^2 c}{T} \left\{ \frac{K(c) - P(c)}{[(a+b)^2 - c^2]\,[(b-a)^2 - c^2]} \right. \\ & \left. + \frac{1}{4ab} \left[\frac{K(a+b) - P(a+b)}{[(a+b)^2 - c^2]} - \frac{K(|a-b|) - P(|a-b|)}{[(a-b)^2 - c^2]} \right] \right\}, \end{aligned} \tag{2.18}$$

where

$$K(x) = \left[\psi\left(1 + \frac{x}{2T\Delta}\right) - \psi\left(\tfrac{1}{2} + \frac{x}{2T\Delta}\right) \right] [B - x^2 A], \tag{2.19}$$

$$P(x) = \frac{T \cdot \Delta}{x} (B - x^2 A), \tag{2.20}$$

$$B = [b^2 - a^2] \left[b\psi'\left(\tfrac{1}{2} + \frac{a}{2T\Delta}\right) - a\psi'\left(\tfrac{1}{2} + \frac{b}{2T\Delta}\right) \right], \tag{2.21}$$

$$A = b\psi'\left(\tfrac{1}{2} + \frac{a}{2T\Delta}\right) + a\psi'\left(\tfrac{1}{2} + \frac{b}{2T\Delta}\right), \tag{2.22}$$

$$T = \frac{\pi}{\beta\Delta}, \qquad u = U/\pi\Delta. \tag{2.23}$$

ψ stands for the digamma function.

3. *Results and discussion*

The right hand side of (2.15) is presented in Fig. 1 as a function of reduced temperature T for different values of μ^2. Since we want to obtain marked changes with temperature without integrating over the thermal Fermi window we use the value $u = 3$ for which the second order perturbation treatment is still valid [10]. The case $\Delta/D = 1$ is the most important for us since this corresponds to the situation independent of band shape. We are dealing with the resonant level composed from band and extra-orbitals and for $\mu^2 = 0$ or 1 we derive the Anderson or Wolff type behaviour. It is apparent from Fig. 1a that in the intermediate region of the values of μ^2 the temperature dependence at low temperatures can be significantly weaker than that for $\mu^2 = 0$ or 1. A quite pronounced minimum can also appear. These effects are quenched with the increase of Δ/D. One can state that the general features observed in Fig. 1 remain in agreement with the properties of dilute Rh-based alloys (as mentioned in [3]). There are also systems for which the impurity contribution to electrical resistivity is temperature independent at low temperatures (AlTi AlV and many others, see [11] for details). Furthermore one can suppose that the non-orthogonality can contribute to the minimum in the electrical resistivity which in general is considered as being due to the addition of the phonon part or taking the crystalline field effects into account. There are systems (e.g. PdPr) in which the minimum appears in the impurity contribution and it is not clear if this effect can be explained through the use of the crystalline field theory [12]. Although the host enhancement does not seem to be important for transport properties (if qualitative conclusions are to be drawn), the applicability of the single level model to a system like PdPr is doubtful. The method of calculations should be also improved. Thus, the present results can stand as a suggestion only that the non-orthogonality can lead to interesting effects in some dilute alloy systems.

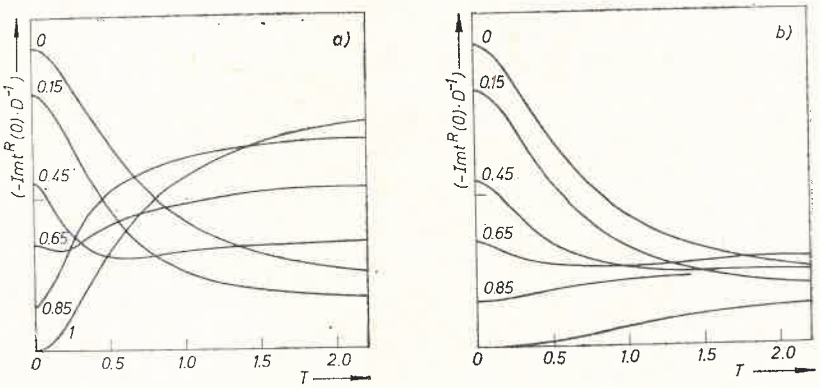

Fig. 1. Imaginary part of the t-matrix as a function of reduced temperature. The numbers by the curves show the values of μ^2. For both cases $u = 3$ is assumed. In a) $\Delta/D = 1$, in b) $\Delta/D = 1/3$

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