EFFECT OF ORDINARY SCATTERING ON THE RESISTIVITY OF DILUTE MAGNETIC ALLOYS

By B. Kozarzewski

Department of Theoretical Physics, Silesian University, Katowice*

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The ordinary and exchange scattering of conduction electrons by magnetic impurities is investigated by using the Nagaoka–Hamman scheme. The solution for the t-matrix, correct in whole temperature range, is found. The resistivity of dilute alloys is calculated.

1. *Introduction*

It is well known that the scattering amplitude of conduction electrons in the presence of a magnetic impurity exhibits a logarithmic divergence at zero temperature. This anomaly has been the object of a considerable number of studies. Most of them are concerned with the exchange scattering only. Recently Kondo [1] has considered the effect of ordinary scattering on the resistivity, but his result is valid at temperatures greater than critical only, and says nothing about the important region around and below T_K.

Our approach is similar to that which had been used by Hamman [2]. He showed that the equations of motion for the thermodynamic Green's functions can be reduced to a single integral equation for the one-electron t-matrix. Such reduction is also possible when ordinary scattering is taken into account. We do it in Section 2. In Section 3., following Zittartz and Müller–Hartman [3] we have solved exactly an integral equation obtained in this manner. In Section 4 an approximation is made and resistivity is calculated.

2. *Green's functions*

We start with the Hamiltonian of free electrons interacting with a single magnetic impurity at the origin of the coordinates

$$H = \sum_{k} \varepsilon_k C^+_{ks} C_{ks} + \frac{V}{N} \sum_{k,k'} C^+_{ks} C_{k's} - \frac{I}{N} \sum_{k,k'} \boldsymbol{\sigma}_{ss'} \cdot \boldsymbol{S} C^+_{ks} C_{k's'} \tag{2.1}$$

(summation over repeated spin indices is assumed).

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* Address: Katedra Fizyki Teoretycznej, Uniwersytet Śląski, Katowice, Bankowa 12, Polska.

The necessary Green's functions are

$$G_{kk'}(\tau-\tau') = -\frac{1}{2}\langle TC_{k's}(\tau)C^+_{ks}(\tau')\rangle \tag{2.2}$$

and

$$\Gamma_{kk'}(\tau-\tau') = -\frac{1}{2}\langle TC_{k's'}(\tau)\boldsymbol{\sigma}_{ss'}\cdot \mathbf{S}C^+_{ks}(\tau')\rangle. \tag{2.3}$$

The equations of motion for their Fourier components can be written, after Nagaoka's decoupling [4], as

$$(z-\varepsilon_{k'})G_{kk'}(z) = \delta_{kk'} + \frac{V}{N}\sum_l G_{kl}(z) - \frac{I}{N}\sum_l \Gamma_{kl}(z), \tag{2.4}$$

$$(z-\varepsilon_{k'})\Gamma_{kk'}(z) = \frac{V}{N}\sum_l \Gamma_{kl}(z) - \frac{I}{N}[S(S+1)-m_{k'}]\sum_l G_{kl}(z) + \frac{I}{N}(1-2n_{k'})\sum_l \Gamma_{kl}(z) \tag{2.5}$$

where

$$z = i\omega_n = i\frac{2n+1}{\beta}\pi,$$

$$n_k = \frac{1}{2}\sum_l \langle C^+_{ls}C_{ks}\rangle = \frac{1}{\beta}\sum_{l,\omega_n} e^{i\omega_n\delta}G_{lk}(i\omega_n) \equiv \sum_l \mathcal{F}_\omega\{G_{lk}(i\omega_n)\}, \tag{2.6a}$$

$$m_k = \sum \langle C^+_{ls}C_{ks'}\,\boldsymbol{\sigma}_{ss'}\cdot\mathbf{S}\rangle = 2\sum_l \mathcal{F}_\omega\{\Gamma_{lk}(i\omega_n)\}. \tag{2.6b}$$

Eqs (2.4) and (2.5) have a formal solution which may be written as

$$G_{kk'}(z) = \frac{\delta_{kk'}}{z-\varepsilon_{k'}} + \frac{1}{N}\frac{t(z)}{(z-\varepsilon_k)(z-\varepsilon_{k'})}, \tag{2.7}$$

where

$$t(z) = \frac{V}{1-VF(z)} - \frac{I^2\Gamma(z)}{(1-VF(z))^2\left(1-VF(z)+2IG(z)+I^2\dfrac{F(z)\Gamma(z)}{1-VF(z)}\right)}, \tag{2.8}$$

$$F(z) = \frac{1}{N}\sum_k \frac{1}{z-\varepsilon_k}, \tag{2.9a}$$

$$G(z) = \frac{1}{N}\sum_k \frac{n_k-\dfrac{1}{2}}{z-\varepsilon_k}, \tag{2.9b}$$

$$\Gamma(z) = \frac{1}{N}\sum_k \frac{m_k-S(S+1)}{z-\varepsilon_k}. \tag{2.9c}$$

To obtain an integral equation for $t(z)$ we must express $G(z)$ and $\Gamma(z)$ as functionals of t. Using Eqs (2.6a), (2.9a) and (2.9b) we have

$$G(z) = R(z) + \mathcal{F}_\omega \left\{ \frac{F(i\omega_n) - F(z)}{z - i\omega_n} F(i\omega_n) t(i\omega_n) \right\}, \tag{2.10}$$

where

$$R(z) = \mathcal{F}_\omega \left\{ \frac{F(i\omega_n) - F(z)}{z - i\omega_u} \right\} - \frac{1}{2} F(z). \tag{2.11}$$

In a similar way from Eqs (2.6b) and (2.9c) we get

$$\Gamma(z) = -\frac{2}{I} \mathcal{F}_\omega \left\{ \frac{F(i\omega_n) - F(z)}{z - i\omega_n} (1 - VF(i\omega_n)) t(i\omega_n) \right\} +$$

$$+ 2\frac{V}{I} R(z) + \left[\frac{V}{I} + S(S+1) \right] F(z). \tag{2.12}$$

Now if we substitute (2.11) and (2.12) in to Eq. (2.8) then we find after simple algebraic computations,

$$t(z) = \frac{V + I_1 F(z) + 2I \mathcal{F}_\omega \left\{ \frac{F(i\omega_n) - F(z)}{z - i\omega_n} t(i\omega_n) \right\}}{1 - 2VF(z) + 2IR(z) - I_1 F^2(z) + 2I \mathcal{F}_\omega \left\{ \frac{[F(i\omega_n) - F(z)]^2}{z - i\omega_n} t(i\omega_n) \right\}}, \tag{2.13}$$

where

$$I_1 = I^2 S(S+1) - IV - V^2.$$

This integral equation becomes identical to Hamman's when $V = 0$.

3. *Solution of integral equation*

To solve Eq. (2.13) we follow a method of Zittartz and Müller-Hartman. First of all we introduce a density of states function $\varrho(z)$, analytical in a neighbourhood of the real axis and normalized to unity at $\varepsilon = 0$. Then Eq. (2.9a) becomes

$$F(z) = \frac{\varrho_0}{N} \int_{-\infty}^{\infty} \frac{\varrho(\omega)}{z - \omega} d\omega. \tag{3.1}$$

Now we can define the retarded and advanced t-matrices; t_r and t_a as given by (2.13) with $F(z)$ replaced by $F_r(z)$ and $F_a(z)$ respectively. These matrices obey two integral equations that can be brought down to the form

$$1 \mp 2\pi i \varrho(z) t_{r,a} = \frac{X(z)}{\Phi_{r,a}(z)}, \tag{3.2}$$

where

$$X(z) = 1 - V[F_r(z) - F_a(z)] + 2IR(z) - I_1 F_r(z) F_a(z) + 2I\chi(z) \tag{3.3}$$

and

$$\Phi_{r,a}(z) = 1 - 2V F_{r,a}(z) + 2IR(z) - I_1 F^2_{r,a}(z) + 2I\varphi_{r,a}(z). \tag{3.4}$$

Functions $\chi(z)$ and $\varphi_{r,a}(z)$ include summation over ω_n, which can be expressed as a contour integral bent round to the real axis yielding

$$\chi(z) = \frac{1}{4\pi i}\int_{-\infty}^{\infty} d\omega \frac{\operatorname{th}\frac{\beta\omega}{2}}{z-\omega}\{[F_r(\omega)-F_r(z)]\,[F_r(\omega)-$$

$$-F_a(z)t_r(\omega)-[F_a(\omega)-F_a(z)]\,[F_a(\omega)-F_r(z)]t_a(\omega)\} \tag{3.5}$$

and

$$\varphi_{r,a}(z) = \frac{1}{4\pi i}\int_{-\infty}^{\infty} d\omega \frac{\operatorname{th}\frac{\beta\omega}{2}}{z-\omega}\{[F_r(\omega)-F_{r,a}(z)]^2 t_r(\omega)-[F_a(\omega)-F_{r,a}(z)]^2 t_a(\omega)\}. \tag{3.6}$$

The details of further calculation are very similar to those of Ref. [3]. The purpose of it is to prove, using Eqs (3.3) to (3.6), the following equation, valid in the neighbourhood of the real axis,

$$\Phi_r^+(z)\Phi_a^-(z) = K(z) \tag{3.7}$$

where

$$K(z) = X^+(z)\,X^-(z) - I[S(S+1)-V]\,[F_r(z)-F_a(z)]^2. \tag{3.8}$$

Here superscripts + or − denote functions analytic in the region including the upper or lower half plane plus neighbourhood of the real axis.

The solution of Eq. (3.7) is

$$\Phi_r^+(z) = e^{-Q^+(z)},\ \Phi_a^-(z) = e^{Q^-(z)},$$

where $Q^+(z)$ and $Q^-(z)$ are upper and lower half plane values of one analytic function

$$Q(z) = \frac{1}{2\pi i}\int_{-\infty}^{\infty} \frac{d\omega}{z-\omega} \ln K(\omega). \tag{3.9}$$

Inserting above solutions in to Eq. (3.2) one obtains

$$1+[F_r(z)-F_a(z)]t_r(z) = X^+(z)\,K^{-\frac{1}{2}}(z)e^{-if(z)}, \tag{3.10a}$$

$$1-[F_r(z)-F_a(z)]t_a(z) = X^-(z)\,K^{-\frac{1}{2}}(z)e^{+if(z)}, \tag{3.10b}$$

where

$$f(z) = \frac{P}{2\pi}\int_{-\infty}^{\infty} \frac{d\omega}{z-\omega} \ln K(\omega). \tag{3.11}$$

Equations (3.10) are again, in principle, integral (but nonsingular) equations, as unknown functions t_r and t_a enter the right hand side *via* $\chi(z)$. We can omit this difficulty if we restrict ourselves to the Lorentzian density of states function.

4. *Resistivity*

According to the above mentioned statement we assume that

$$\varrho(z) = \frac{D^2}{z^2+D^2}. \tag{4.1}$$

Then

$$F_{r,a}(z) = \frac{\pi\varrho_0}{N}\frac{D}{z\pm iD}, \tag{4.2}$$

and from Eq. (2.11) we get

$$R^{\pm}(z) = \frac{\varrho_0}{N}\varrho(z)\left[\psi\left(\frac{1}{2}+\frac{\beta D}{2\pi}\right)-\psi\left(\frac{1}{2}\pm\frac{\beta z}{2\pi i}\right)\right], \tag{4.3}$$

where $\psi(z)$ is the digamma function.
By use of the above results Eq. (3.5) is reduced to

$$\chi(z) = -\frac{\pi^2\varrho_0}{N}\varrho(z)(A-zB), \tag{4.4}$$

where

$$A = \frac{\varrho_0}{4\pi Ni}\int_{-\infty}^{\infty} d\omega \,\mathrm{th}\,\frac{\beta\omega}{2}\frac{\omega+2iD}{(\omega+iD)^2}[t_r(\omega)-t_a(-\omega)]$$

and

$$B = \frac{\varrho_0}{4\pi Ni}\int_{-\infty}^{\infty} d\omega \,\mathrm{th}\,\frac{\beta\omega}{2}\frac{t_r(\omega)+t_a(-\omega)}{(\omega+iD)^2}$$

are constants of order $\Gamma^2 = \left(\frac{V\varrho_0}{N}\right)^2$ and Γ respectively. Now we can evaluate the functions $X^{\pm}(z)$, they are

$$X^{\pm}(z) = 1+\varrho(z)\left\{\gamma\left[\psi\left(\frac{1}{2}+\frac{\beta D}{2\pi}\right)-\psi\left(\frac{1}{2}\pm\frac{\beta z}{2\pi i}\right)\right]-\right.$$
$$\left.-\pi^2[\gamma^2 S(S+1)-\Gamma\gamma-\Gamma^2+\gamma(A-zB)]-2\pi\Gamma\frac{\omega}{D}\right\}, \tag{4.5}$$

In the case of antiferromagnetic exchange ($\gamma = I\varrho_0/N < 0$) the Kondo temperature T_K is determined from the relation

$$X^{+}(0) = 0.$$

In our case it equals

$$kT_K = \frac{2\alpha D}{\pi}\exp\left\{\frac{1+(\pi\Gamma)^2}{2\gamma}+\pi^2\left[\frac{\Gamma}{2}-S(S+1)\frac{\gamma}{2}-A\right]\right\}, \tag{4.6}$$

where we have used the well known relations $\psi(1/2) = -\ln 4\alpha$ and $\psi(x) \approx \ln x$ for $x \gg 1$. The presence of the three last terms in the exponent makes our T_K different from the result of Ref. [1].

Our next task is to obtain the explicit form of the function $f(z)$. We were able to find it in an approximated way only. When we use Eqs (3.3) and (3.8) dropping terms of order γ we get.

$$f(z) = i \ln \frac{1-VF_r(z)}{1-VF_a(z)}.$$

Introducing this into (3.10a) we have finally

$$t_r(\omega) = \frac{1}{2\pi i \varrho_0 \varrho(\omega)} \left\{ 1 - \frac{1-VF_r(\omega)}{1-VF_a(\omega)} \times \right.$$

$$\left. \times \frac{X^+(\omega)}{\left[X^+(\omega)X^-(\omega) + \pi^2\gamma^2\varrho^2(\omega) \left(S(S+1) - \frac{\Gamma}{\gamma} \right) \right]^{1/2}} \right\}. \quad (4.7)$$

Taking into account that the relaxation time of the conduction electrons is given by

$$[2\tau(\omega)]^{-1} = c \operatorname{Im} t_r(\omega),$$

we find for the resistivity

$$R = \frac{3c}{2\pi\varrho_0^2 e^2 v_F^2} \left\{ 1 - \frac{1-\pi^2\Gamma^2}{1+\pi^2\Gamma^2} \ln \frac{T}{T_K} \left[\ln^2 \frac{T}{T_K} + \pi^2 \left(S(S+1) - \frac{\Gamma}{\gamma} \right) \right]^{-\frac{1}{2}} \right\}. \quad (4.8)$$

This becomes identical to Hamman's result when $\Gamma = 0$. A comparison with Kondo's high temperature approximation can be made when we assume $T \gg T_K$ and expand (4.9) into a powers of $1/\ln \frac{T}{T_K}$. Then to the second order we get formula

$$R = \frac{3c}{\pi e^2 \varrho_0^2 v_F^2} \left[\sin^2 \eta + \frac{\pi^2}{4} \left(S(S+1) - \frac{\Gamma}{\gamma} \right) \cos 2\eta \ln^{-2} \frac{T}{T_K} \right]$$

$$(\operatorname{tg} \eta = \pi\Gamma),$$

which differs somewhat from that of Ref. [1].

The solution (3.10) can be used as a starting point for the calculation of other measurable quantities, *e. g.*, specific heat or thermoelectric power. This last quantity seems to be very interesting as the giant thermoelectric power of dilute magnetic alloys is, in Kondo's opinion, a result of a cooperation of ordinary and exchange scattering.

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