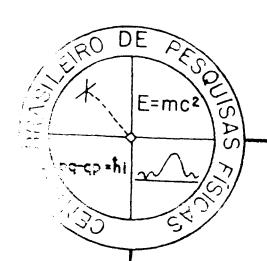
### NOTAS DE FÍSICA



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### ON THE SPIN DISORDER RESISTIVITY \*

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#### ABSTRACT

An extension of the calculation of the temperature independent resistivity performed by Blackman and Elliott is presented, in order to describe transition metal-like hosts. A Dyson-like equation is derived for the one-electron s-propagator. Then, only terms to second order in the exchange parameters, in absence of magnetic order, are considered. Ar expression for the temperature independent resistivity is obtained in terms of phase-shifts and exchange couplings.

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#### 1. INTRODUCTION

It is well known that a magnetic rare-earth impurity embedded in a transition metal environment interacts with both the s and d conduction states. The potential introduced by the impurity has a spin independent and a spin dependent part. The spin independent potential arises from the charge difference introduced by the impurity, the source of spin dependent scattering being the exchange coupling to the localized moment.

Since Kondo's work (1964) 1, one relates the spin dependent scattering to the internal degree of freedom of the spin. In that paper Kondo calculated the resistivity due to the exchange interaction to third order in the exchange parameters, showing then the existence of a singular temperature dependence. A more complete theory, based on the Green function formalism had been given by Nagaoka (1965) 2, Hamann and Bloomfield (1967) 3. Blackman and Elliott (1969) 4 calculated the resistivity due to a small concentration of magnetic impurities on a single band, taking into account also the effects of the charge difference introduced by the impurity. It is the purpose of our calculation to extend the work of Blackman and Elliott in order to include a more complicated band structure, namely a transition metal host which exhibits s and d-like bands. The plan of this paper is as follows: in Sec..II we formulate the problem under the basic assumption that charge screening is entirely performed by the d-electrons and s-d hybridization induced by the impurity takes place only at the impurity site. Since conduction is due almost exclusively to the s-electrons, we restrict ourselves to the derivation of a Dyson-like equation for the oneelectron s-propagator in terms of the host metal propagators. This equation is valid to all orders in perturbation theory within the accuracy of

Nagaoka's decoupling scheme. In Sec. III the equation for the one-electron s-propagator is solved to second order in the exchange parameters  $J^{(s)}$  and  $J^{(d)}$ . This solution enable us to compute the temperature independent resistivity in terms of the exchange couplings and the phase-shifts introduced by the spin independent potential.

Finally, in the discussions, we compare briefly the obtained results to the usual ones where the effect of spin independent potential is neglected. From that comparison and effective exchange coupling can be defined. The third order terms (Kondo effects) will be discussed in a forthcoming paper.

#### II. FORMULATION OF THE PROBLEM

#### a) HAMILTONIAN OF THE SYSTEM

We consider a two band picture for the host, consisting of s and d bands, which for simplicity are not hybridized. Since conduction is mostly performed by s-electrons, we restrict our calculation to quantities such as the  $G_{ij}^{SS}(\omega)$  propagator.

The pure host Hamiltonian is:

$$\mathcal{H}_{c} = \sum_{i,j\sigma} \tau_{ij}^{(s)} c_{i\sigma}^{+} c_{j\sigma} + \sum_{i,j\sigma} \tau_{ij}^{(d)} d_{i\sigma}^{+} d_{j\sigma}$$
(1)

The impurity, placed at the origin, contributes two sources of scattering:

(i) Potencial scattering through d-d scattering and impurity induced s-d mixing. Then:

$$\mathcal{H}_{pot}^{imp} = V_{dd} \sum_{\sigma} n_{o\sigma}^{(d)} + \sum_{\sigma} \{V_{sd} c_{o\sigma}^{\dagger} c_{o\sigma} + V_{ds} d_{o\sigma}^{\dagger} c_{o\sigma}\}$$
 (2)

The Hamiltonian (2) has already been used (Gomes, Thesis Paris, 1967  $^5$ ) but it is rather a simplified version of the convenient one (cf. Riedinger and Gautier, 1970  $^6$ ). However, due to its simplicity, we conserve it in this calculation, expecting that the main physical aspects are described properly. Furthermore, we neglect completely intra s-band scattering  $V_{ss}$ , assuming that screening is performed by the d's.

ii) Spin scattering - conduction electrons are coupled to the impurity spin through:

where the spin components of conduction electrons are defined by:

$$\sigma_{i}^{z} = a_{i\uparrow}^{+} a_{i\uparrow} - a_{i\downarrow}^{+} a_{i\downarrow}$$

$$\sigma_{i}^{+} = a_{i+}^{+} a_{i+}$$

$$\sigma_i^- = a_{i\downarrow}^+ a_{i\uparrow}$$

The  $a_i$ 's in the above expression stand for the  $c_i$  or  $d_i$ , according to s and d states respectively.

The total Hamiltonian for the alloy is:

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{pot}^{imp} + \mathcal{H}_{exch}^{imp}$$
 (4)

This Hamiltonian intends to be a model for rare-earths diluted in transi-

tion-metal-like host or intermetallic compounds. Potential scattering (which may be rather strong), arises from the difference of valence between host and the trivalent rare-earth.

b) SOLUTION OF THE PROBLEM IN THE ABSENCE OF SPIN SCATTERING

(b.i) PURE HOST SOLUTION  $(\mathcal{X} = \mathcal{Y}_0)$ 

We firstly derive simple results that will be useful later on; by introducing the pure host propagators:

$$P_{1j}^{ss}(\omega) = \langle c_{1\sigma}; c_{j\sigma}^{+} \rangle \omega$$

$$P_{ij}^{dd}(\omega) = \langle d_{i\sigma}; d_{j\sigma}^+ \rangle_{\omega}$$

it follows from the usual equations of motion:

$$\omega P_{ij}^{ss}(\omega) = \frac{1}{2\pi} \delta_{ij} + \sum_{\ell} T_{i\ell}^{(s)} P_{\ell j}^{ss}(\omega)$$

$$\omega P_{ij}^{dd}(\omega) = \frac{1}{2\pi} \delta_{ij} + \sum_{\ell} T_{i\ell}^{(d)} P_{\ell j}^{dd}(\omega)$$
(5)

The trivial solutions are:

$$P_{kk}^{ss}(\omega) = \frac{1}{2\pi} \frac{\delta_{kk'}}{\omega - \epsilon_k(s)}$$
 and  $P_{kk'}^{dd}(\omega) = \frac{1}{2\pi} \frac{\delta_{kk'}}{\omega - \epsilon_k(d)}$  (6-a)

or in the Wannier representation:

$$P_{ij}^{ss}(\omega) = \frac{1}{2\pi} \sum_{k} \frac{e^{ik \cdot (R_i - R_j)}}{\omega - \varepsilon_k^{(s)}} \quad \text{and} \quad P_{ij}^{dd}(\omega) = \frac{1}{2\pi} \sum_{k} \frac{e^{ik \cdot (R_i - R_j)}}{\omega - \varepsilon_k^{(d)}}$$
(6-b)

(b.ii) SOLUTION FOR THE PROBLEM DEFINED BY \$\mathbb{H}\_0 + \mathbb{H}\_{pot}^{imp}\$
To do that we introduce the notation:

$$G_{ij}^{ss}(\omega) = \langle c_{i\sigma}; c_{j\sigma}^{\dagger} \rangle_{\omega}; \qquad G_{ij}^{ds}(\omega) = \langle d_{i\sigma}; c_{j\sigma}^{\dagger} \rangle_{\omega}$$

$$G_{ij}^{dd}(\omega) = \langle d_{i\sigma}; d_{j\sigma}^{+} \rangle_{\omega}; \qquad G_{ij}^{sd}(\omega) = \langle c_{i\sigma}; d_{j\sigma}^{+} \rangle_{\omega}$$

Due to impurity induced s-d mixing one now has pairs of coupled equations.

DETERMINATION OF THE  $G_{ij}^{ss}(\omega)$  AND  $G_{ij}^{ds}(\omega)$  PROPAGATORS

From the general equation of motion:

$$\omega G_{ij}^{ss}(\omega) = \frac{1}{2\pi} \delta_{ij} + \sum_{\ell} T_{i\ell}^{(s)} G_{\ell j}^{ss}(\omega) + \delta_{io} V_{sd} G_{oj}^{ds}(\omega)$$
 (7.a)

$$\omega G_{ij}^{ds}(\omega) = \sum_{\ell} T_{i\ell}^{(d)} G_{\ell,i}^{ds}(\omega) + \delta_{io} V_{dd} G_{o,i}^{ds}(\omega) + \delta_{io} V_{ds} G_{o,i}^{ss}(\omega)$$
 (7.6)

Fourier transforming equations (7) and after some algebraic manipulations, one gets the results:

$$G_{kk}^{SS}(\omega) = \frac{1}{2\pi} \frac{\delta_{kk'}}{\omega - \varepsilon_k^{(S)}} + \frac{1}{2\pi} \frac{1}{\omega - \varepsilon_k^{(S)}} T^{SS}(\omega) \frac{1}{\omega - \varepsilon_k^{(S)}}$$
(8.a)

and

$$G_{kk}^{ds}(\omega) = \frac{1}{2\pi} \frac{1}{\omega - \varepsilon_{k}^{(d)}} T^{ds}(\omega) \frac{1}{\omega - \varepsilon_{k}^{(s)}}$$
(8.b)

where the  $T(\omega)$  matrices are defined as:

$$T^{SS}(\omega) = \frac{|V_{Sd}|^2 P_{OO}^{dd}(\omega)}{1 - V_{dd} P_{OO}^{dd}(\omega) - |V_{Sd}|^2 P_{OO}^{SS}(\omega) P_{OO}^{dd}(\omega)}$$
(8.c)

$$T^{ds}(\omega) = \frac{V_{ds}}{1 - V_{dd} P_{oo}^{dd}(\omega) - |V_{sd}|^2 P_{oo}^{ss}(\omega) P_{oo}^{dd}(\omega)}$$
(8.d)

In the Wannier representation equations (8.a) and (8.b) can be rewritten as:

$$G_{ij}^{SS}(\omega) = P_{ij}^{SS}(\omega) + 2\pi P_{io}^{SS}(\omega) T^{SS}(\omega) P_{oj}^{SS}(\omega)$$
 (9.a)

$$G_{ij}^{ds}(\omega) = 2\pi P_{io}^{dd}(\omega) T^{ds}(\omega) P_{oj}^{ss}(\omega)$$
(9.b)

DETERMINATION OF THE  ${\sf G_{ij}^{dd}}(\omega)$  AND  ${\sf G_{ij}^{sd}}(\omega)$  PROPAGATORS

Again, from the equations of motion:

$$\omega G_{ij}^{dd}(\omega) = \frac{1}{2\pi} \delta_{ij} + \sum_{\ell} T_{i\ell}^{(d)} G_{\ell j}^{dd}(\omega) + \delta_{io} V_{dd} G_{oj}^{dd}(\omega) + \delta_{io} V_{ds} G_{oj}^{sd}(\omega)$$
 (10.a)

$$\omega G_{ij}^{sd}(\omega) = \sum_{k} T_{ik}^{(s)} G_{kj}^{sd}(\omega) + \delta_{io} V_{sd} G_{oj}^{dd}(\omega)$$
 (10.b)

Proceeding exactly as in the above case one obtains:

$$G_{kk'}^{dd}(\omega) = \frac{1}{2\pi} \frac{\delta_{kk'}}{\omega - \varepsilon_{k}^{(d)}} + \frac{1}{2\pi} \frac{1}{\omega - \varepsilon_{k}^{(d)}} T^{dd}(\omega) \frac{1}{\omega - \varepsilon_{k'}^{(d)}}$$
(10.c)

and

$$G_{kk'}^{sd}(\omega) = \frac{1}{2\pi} \frac{1}{\omega - \varepsilon_k^{(s)}} T^{sd}(\omega) \frac{1}{\omega - \varepsilon_k^{(d)}}$$
(10.d)

where the new  $T(\omega)$  matrices are defined as:

$$T^{dd}(\omega) = \frac{V_{dd} + |V_{sd}|^2 P_{oo}^{SS}(\omega)}{1 - V_{dd} P_{oo}^{dd}(\omega) - |V_{sd}|^2 P_{oo}^{SS}(\omega) P_{oo}^{dd}(\omega)}$$
(10.e)

$$T^{sd}(\omega) = \frac{V_{sd}}{1 - V_{dd} P_{oo}^{dd}(\omega) - |V_{sd}|^2 P_{oo}^{ss}(\omega) P_{oo}^{dd}(\omega)}$$
(10.f)

In the Wannier representation, these propagators read:

$$G_{i,j}^{dd}(\omega) = P_{i,j}^{dd}(\omega) + 2\pi P_{i,0}^{dd}(\omega) T^{dd}(\omega) P_{0,j}^{dd}(\omega)$$
 (11.a)

and

$$G_{i,i}^{sd}(\omega) = 2\pi P_{i,o}^{ss}(\omega) T^{sd}(\omega) P_{o,i}^{dd}(\omega)$$
 (11.b)

Therefore, the impurity problem in the absence of spin scattering, is completely solved by equations (9.a), (9.b), (11.a), (11.b) in terms of  $V_{\rm dd}$ ,  $V_{\rm sd}$  and  $V_{\rm ds}$ .

#### c) INTEGRAL EQUATION FOR THE COMPLETE HAMILTONIAN

Now we start discussing the complete problem including exchange. Introducing the notation:

$$\Gamma_{ij}^{ss}(\omega) = \langle \langle c_{i\sigma}; c_{j\sigma}^{+} \rangle \rangle_{\omega} ; \qquad \Gamma_{ij}^{ds}(\omega) = \langle \langle d_{i\sigma}; c_{j\sigma}^{+} \rangle \rangle_{\omega}$$

$$\Theta_{ij}^{ss}(\omega) = \langle \langle \sigma c_{i\sigma} S_{o}^{z} + c_{i-\sigma} S_{o}^{-\sigma}; c_{j\sigma}^{+} \rangle \rangle_{\omega}$$

$$\Theta_{ij}^{ds}(\omega) = \langle \langle \sigma d_{i\sigma} S_{o}^{z} + d_{i-\sigma} S_{o}^{-\sigma}; c_{j\sigma}^{+} \rangle \rangle_{\omega}$$

one gets, from the general equation of motion: (it should be noted that we are only interested in s-s propagators)

$$\omega \Gamma_{ij}^{ss}(\omega) = \frac{1}{2\pi} \delta_{ij} + \sum_{\ell} T_{i\ell}^{(s)} \Gamma_{\ell j}^{ss}(\omega) + \delta_{io} V_{sd} \Gamma_{oj}^{ds}(\omega) + J^{(s)} \delta_{io} \Theta_{oj}^{ss}(\omega)$$
 (12.a) and

$$\omega \Gamma_{ij}^{ds}(\omega) = \sum_{\ell} T_{i\ell}^{(d)} \Gamma_{\ell j}^{ds}(\omega) + \delta_{io} V_{dd} \Gamma_{oj}^{ds}(\omega) + \delta_{io} V_{ds} \Gamma_{oj}^{ss}(\omega) + J^{(d)} \delta_{io} \Theta_{oj}^{ds}(\omega)$$

$$(12.b)$$

These two exact equations of motion completely specify the propagators  $\Gamma_{i,j}^{ss}(\omega)$  and  $\Gamma_{i,j}^{ds}(\omega)$  in terms of the "spin flip" propagators  $\Theta_{i,j}(\omega)$ .

Now we can obtain approximate equations of motion for the  $\Theta_{ij}^{ss}(\omega)$  and  $\Theta_{ij}^{ds}(\omega)$  Green's functions. We follow strictly Blackman and Elliott's procedure  $^{7}$ , decoupling higher order propagators according to Nagaoka's scheme  $^{2}$ ; one gets:

$$\omega \Theta_{ij}^{SS}(\omega) = \frac{1}{2\pi} \sigma < S_{o}^{Z} > \delta_{ij} + \sum_{\ell} T_{i\ell}^{(s)} \Theta_{\ell j}^{SS}(\omega) + \delta_{io} V_{sd} \Theta_{oj}^{ds}(\omega) +$$

$$+ J^{(s)} \{S_{o}(S_{o}+1)\delta_{io} \Gamma_{oj}^{SS}(\omega) - \delta_{io} \Theta_{oj}^{SS}(\omega) + 2\alpha_{io}^{SS}\Theta_{oj}^{SS}(\omega) -$$

$$- 3 \beta_{io}^{SS} \Gamma_{oj}^{SS}(\omega)\} + J^{(d)} \{2\alpha_{io}^{Sd} \Theta_{oj}^{ds}(\omega) - 3 \beta_{io}^{Sd} \Gamma_{oj}^{ds}(\omega)\}$$

$$(13.a)$$

and

$$\omega \Theta_{ij}^{ds}(\omega) = \sum_{\ell} T_{i\ell}^{(d)} \Theta_{\ell j}^{ds}(\omega) + \delta_{io} V_{dd} \Theta_{oj}^{ds}(\omega) + \delta_{io} V_{ds} \Theta_{oj}^{ss}(\omega) +$$

$$+ J^{(s)} \left\{ 2 \alpha_{io}^{ds} \Theta_{oj}^{ss}(\omega) - 3 \beta_{io}^{ds} \Gamma_{oj}^{ss}(\omega) \right\} +$$

$$+ J^{(d)} \left\{ S_{o}(S_{o}+1) \delta_{io} \Gamma_{oj}^{ds}(\omega) - \delta_{io} \Theta_{oj}^{ds}(\omega) + 2 \alpha_{io}^{dd} \Theta_{oj}^{ds}(\omega) -$$

$$- 3 \beta_{io}^{dd} \Gamma_{oj}^{ds}(\omega) \right\}$$

$$(13.b)$$

Where the correlation functions  $\alpha$  and  $\beta$  are defined as:

$$\alpha_{ij}^{ss} = \langle c_{i\sigma}^{+} c_{j\sigma} \rangle \qquad \alpha_{ij}^{dd} = \langle d_{i\sigma}^{+} d_{j\sigma} \rangle 
\alpha_{ij}^{sd} = \langle c_{i\sigma}^{+} d_{j\sigma} \rangle \qquad \alpha_{ij}^{ds} = \langle d_{i\sigma}^{+} c_{j\sigma} \rangle \qquad (14)$$

$$\beta_{io}^{ss} = \langle c_{i\sigma}^{+} c_{i-\sigma} S_{o}^{-\sigma} \rangle \qquad \beta_{io}^{dd} = \langle d_{i\sigma}^{+} d_{i-\sigma} S_{o}^{-\sigma} \rangle 
\beta_{io}^{sd} = \langle a_{i\sigma}^{+} c_{i-\sigma} S_{o}^{-\sigma} \rangle \qquad \beta_{io}^{ds} = \langle c_{i\sigma}^{+} d_{i-\sigma} S_{o}^{-\sigma} \rangle$$

It is clear that equations (12) and (13) completely determine the propagator  $\Gamma_{ij}^{ss}(\omega)$ . The rest of this paragraph will be used in casting these equations in the form of an integral equation for  $\Gamma_{ij}^{ss}(\omega)$ .

(c.i) TRANSFORMATION OF EQUATIONS (12) IN TERMS OF THE G PROPAGATORS
Fourier transforming equations (12), one has:

$$(\omega - \varepsilon_{k}^{(s)}) \Gamma_{kk}^{ss}, (\omega) = \frac{1}{2\pi} \delta_{kk}, + V_{sd} \sum_{k''} \Gamma_{k''k}^{ds}, (\omega) + J^{(s)} \sum_{k''} \Theta_{k''k}^{ss}, (\omega)$$
(15.a)

$$(\omega - \varepsilon_{k}^{(d)}) \Gamma_{kk}^{ds} (\omega) = V_{dd} \sum_{k} \Gamma_{k''k}^{ds} (\omega) + V_{ds} \sum_{k''} \Gamma_{k''k}^{ss} (\omega) + J^{(d)} \sum_{k''} \Theta_{k''k}^{ds} (\omega)$$

$$(15.b)$$

Introducing the notation:

$$x_{k'}^{ss}(\omega) = \sum_{k''} \Gamma_{k''k'}^{ss}(\omega)$$
;  $x_{k'}^{ds}(\omega) = \sum_{k''} \Gamma_{k''k'}^{ds}(\omega)$ 

$$y_{k'}^{ss}(\omega) = \sum_{k''} \Theta_{k''k'}^{ss}(\omega)$$
;  $y_{k'}^{ds}(\omega) = \sum_{k''} \Theta_{k''k'}^{ds}(\omega)$ 

it follows from (15):

$$x_{k_{1}}^{SS}(\omega) = \frac{1}{2\pi} \frac{1}{\omega - \varepsilon_{k_{1}}^{(S)}} + V_{Sd} P_{OO}^{SS}(\omega) x_{k_{1}}^{dS}(\omega) + J^{(S)} P_{OO}^{SS}(\omega) y_{k_{1}}^{SS}(\omega)$$
 (16.a)

$$\left\{ 1 - V_{dd} P_{oo}^{dd}(\omega) \right\} x_{k'}^{dd}(\omega) = V_{ds} P_{oo}^{dd}(\omega) x_{k'}^{ss}(\omega) - J^{(d)} P_{oo}^{dd}(\omega) y_{k'}^{ds}(\omega) (16.b)$$

From these equations one is able to make explicit  $x_{k}^{ss}(\omega)$  and  $x_{k}^{ds}(\omega)$  in terms of known quantities and the  $y_{k}^{l}$ .

Using the notation:

$$X(\omega) = 1 - V_{dd} P_{QQ}^{dd}(\omega) - |V_{Sd}|^2 P_{QQ}^{ss}(\omega) P_{QQ}^{dd}(\omega)$$
 (16.c)

one gets:

$$x_{k'}^{ds}(\omega) = \frac{1}{2\pi} \frac{y_{ds} P_{oo}^{dd}(\omega)}{X(\omega)} \frac{1}{\omega - \varepsilon_{k'}^{(s)}} + J^{(s)} \frac{y_{ds} P_{oo}^{dd}(\omega) P_{oo}^{ss}(\omega)}{X(\omega)} y_{k'}^{ss}(\omega) +$$

$$+ J^{(d)} \frac{P_{oo}^{dd}(\omega)}{X(\omega)} y_{k'}^{ds}(\omega)$$
 (16.d)

and

$$x_{k'}^{SS}(\omega) = \frac{1}{2\pi} \left\{ 1 + \frac{|V_{sd}|^2 P_{oo}^{dd}(\omega) P_{oo}^{SS}(\omega)}{X(\omega)} \right\} \frac{1}{\omega - \epsilon_{k'}^{(S)}} +$$

$$+ J(s) \left\{ 1 + \frac{|V_{sd}|^2 P_{oo}^{dd}(\omega) P_{oo}^{ss}(\omega)}{\chi(\omega)} \right\} P_{oo}^{ss}(\omega) y_{k'}^{ss}(\omega) +$$

+ 
$$J^{(d)} = \frac{V_{sd} P_{oo}^{ss}(\omega) P_{oo}^{dd}(\omega)}{X(\omega)} y_{k'}^{ds}(\omega)$$
 (16.c)

Substituting (16.c) and (16.d) into equations (15.a) and (15.b), one has:

$$\Gamma_{kk}^{ss}(\omega) = \frac{1}{2\pi} \left\{ \frac{\delta_{kk'}}{\omega \varepsilon_{k}^{(s)}} + \frac{1}{\omega \varepsilon_{k}^{(s)}} \frac{|V_{sd}|^{2} P_{oo}^{dd}(\omega)}{X(\omega)} \frac{1}{\omega \varepsilon_{k'}^{(s)}} \right\} + \left\{ \frac{1}{\omega \varepsilon_{k}^{(s)}} + \frac{1}{\omega \varepsilon_{k}^{(s)}} \frac{|V_{sd}|^{2} P_{oo}^{dd}(\omega)}{X(\omega)} \sum_{k''} \frac{1}{\omega \varepsilon_{k''}^{(s)}} \right\} J^{(s)} y_{k''}^{ss}(\omega) + \frac{1}{\omega \varepsilon_{k''}^{(s)}} \frac{V_{sd}}{\omega \varepsilon_{k''}^{(s)}} + \frac{1}{\omega \varepsilon_{k''}^{(s)}} \frac{1}{\omega \varepsilon_{k''}^{(s)}} \left\{ J^{(s)} y_{k''}^{ss}(\omega) + \frac{1}{\omega \varepsilon_{k''}^{(s)}} \right\} J^{(s)} y_{k''}^{ss}(\omega) + \frac{1}{\omega \varepsilon_{k''}^{(s)}} \frac{V_{sd}}{\omega \varepsilon_{k''}^{(s)}} \left\{ J^{(s)} y_{k''}^{ss}(\omega) + \frac{1}{\omega \varepsilon_{k''}^{(s)}} \right\} J^{(s)} y_{k''}^{ss}(\omega) + \frac{1}{\omega \varepsilon_{k''}^{(s)}} \frac{V_{sd}}{\omega \varepsilon_{k''}^{(s)}} \left\{ J^{(s)} y_{k''}^{ss}(\omega) + \frac{1}{\omega \varepsilon_{k''}^{(s)}} \right\} J^{(s)} y_{k''}^{ss}(\omega) + \frac{1}{\omega \varepsilon_{k''}^{(s)}} \frac{J^{(s)} y_{k''}^{ss}(\omega)}{\omega \varepsilon_{k''}^{(s)}} + \frac{1}{\omega \varepsilon_{k''}^{(s)}} \frac{J^{(s)} y_{k''}^{ss}(\omega)}{\omega \varepsilon_{k''}^{ss}(\omega)} + \frac{1}{\omega \varepsilon_{k''}^{ss}} \frac{J^$$

$$+ \frac{1}{\omega - \varepsilon_{k}^{(s)}} \frac{v_{sd}}{x(\omega)} \sum_{k''} \frac{1}{\omega - \varepsilon_{k''}^{(d)}} J^{(d)} y_{k'}^{ds}(\omega)$$
 (17.a)

 $\Gamma_{kk}^{ds}(\omega) = \frac{1}{2\pi} \frac{1}{\omega - \varepsilon_{k}^{(d)}} \frac{V_{ds}}{X(\omega)} \frac{1}{\omega - \varepsilon_{k}^{(s)}} + \frac{1}{\omega - \varepsilon_{k}^{(d)}} \frac{V_{ds}}{X(\omega)} \sum_{k} \frac{1}{\omega - \varepsilon_{k}^{(s)}} J^{(s)} y_{k}^{ss}(\omega) + \frac{1}{\omega - \varepsilon_{k}^{(s)}} J^{($ 

$$+\frac{1}{\omega-\varepsilon_{\mathbf{k}}^{(\mathbf{d})}}\left\{1+\frac{V_{\mathbf{d}\mathbf{d}}+|V_{\mathbf{s}\mathbf{d}}|^{2}P_{\mathbf{oo}}^{\mathsf{SS}}(\omega)}{X(\omega)}\sum_{\mathbf{k}''}\frac{1}{\omega-\varepsilon_{\mathbf{k}''}^{(\mathbf{d})}}\right\}J^{(\mathbf{d})}y_{\mathbf{k}'}^{\mathsf{ds}}(\omega) \tag{17.b}$$

Remembering the expressions for the propagators in presence of potential scattering, one gets:

$$\Gamma_{kk'}^{ss}(\omega) = G_{kk'}^{ss}(\omega) + 2\pi \sum_{k_1} G_{kk_1}^{ss}(\omega) J^{(s)} \sum_{k_2} \Theta_{k_2k'}^{ss}(\omega) + 2\pi \sum_{k_1} G_{kk_1'}^{sd}(\omega) J^{(d)} \sum_{k_2} \Theta_{k_2k'}^{ds}(\omega)$$

$$(17.c)$$

and

$$\Gamma_{kk}^{ds}(\omega) = G_{kk}^{ds}(\omega) + 2\pi \sum_{k_1} G_{kk_1}^{ds}(\omega) J^{(s)} \sum_{k_2} G_{k_2k}^{ss}(\omega) + 2\pi \sum_{k_1} G_{kk_1}^{dd}(\omega) J^{(d)} \sum_{k_2} G_{k_2k}^{ds}(\omega)$$

$$(17.d)$$

Finally, in the Wannier representation:

$$\Gamma_{ij}^{ss}(\omega) = G_{ij}^{ss}(\omega) + 2\pi G_{io}^{ss}(\omega) J^{(s)} \Theta_{oj}^{ss}(\omega) + 2\pi G_{io}^{sd}(\omega) J^{(d)} \Theta_{oj}^{ds}(\omega)$$
(18.a)

$$\Gamma_{ij}^{ds}(\omega) = G_{ij}^{ds}(\omega) + 2\pi G_{io}^{ds}(\omega) J^{(s)} \Theta_{oj}^{ss}(\omega) + 2\pi G_{io}^{dd}(\omega) J^{(d)} \Theta_{oj}^{ds}(\omega)$$
(18.b)

Equations (18) complete the first step of the determination of the integral equation for  $\Gamma^{SS}(\omega)$ .

(c.ii) TRANSFORMATION OF EQUATIONS (13) IN TERMS OF THE G-PROPAGATORS

Fourier transforming equations (13) one has:

$$(\omega - \varepsilon_{\mathbf{k}}^{(s)}) \Theta_{\mathbf{k}\mathbf{k}}^{ss}, (\omega) = \frac{1}{2\pi} \sigma \langle S_{\mathbf{0}}^{z} \rangle \delta_{\mathbf{k}\mathbf{k}}^{s}, + V_{sd} y_{\mathbf{k}'}^{ds}(\omega) + Z_{\mathbf{k}\mathbf{k}'}^{ss}, (\omega)$$
 (19.a)

$$(\omega - \varepsilon_k^{(d)}) \Theta_{kk}^{ds} \cdot (\omega) = V_{dd} y_k^{ds} \cdot (\omega) + V_{ds} y_k^{ss} \cdot (\omega) + Z_{kk}^{ds} \cdot (\omega)$$
 (19.b)

where we introduced the notation:

$$Z_{kk}^{ss}(\omega) = J^{(s)} \left\{ S_{0}(S_{0}+1) \times_{k'}^{ss}(\omega) - y_{k'}^{ss}(\omega) + 2 \sum_{k_{1}} \alpha_{kk}^{ss} y_{k'}^{ss}(\omega) - 3 \sum_{k_{1}} \beta_{kk_{1}}^{ss} \times_{k'}^{ss}(\omega) \right\} + J^{(d)} \left\{ 2 \sum_{k_{1}} \alpha_{kk_{1}}^{sd} y_{k'}^{ds}(\omega) - 3 \sum_{k_{1}} \beta_{kk_{1}}^{sd} \times_{k'}^{ds}(\omega) \right\}$$

$$- 3 \sum_{k_{1}} \beta_{kk_{1}}^{sd} \times_{k'}^{ds}(\omega) \right\}$$

$$(19.c)$$

and

$$Z_{kk}^{ds}(\omega) = J^{(s)} \left\{ 2\sum_{k} \alpha_{kk_{1}}^{ds} y_{k'}^{ss}(\omega) - 3\sum_{k_{1}} \beta_{kk_{1}}^{s} x_{k'}^{ss}(\omega) \right\} + J^{(d)} \left\{ S_{0}(S_{0}+1) x_{k'}^{ds}(\omega) - y_{k'}^{ds}(\omega) + 2\sum_{k_{1}} \alpha_{kk_{1}}^{dd} y_{k'}^{ds}(\omega) - 3\sum_{k_{1}} \beta_{kk_{1}}^{dd} x_{k'}^{ds}(\omega) \right\}$$

$$- 3 \sum_{k_{1}} \beta_{kk_{1}}^{dd} x_{k'}^{ds}(\omega) \right\}$$

$$(19.d)$$

Proceeding exactly as before one obtains for the propagators  $\Theta_{kk}^{SS}$ ,  $(\omega)$  and  $\Theta_{kk}^{dS}$ ,  $(\omega)$ :

$$\Theta_{kk}^{SS}(\omega) = \sigma \langle S_0^z \rangle \frac{1}{2\pi} \left\{ \frac{\delta_{kk'}}{\omega - \varepsilon_k^{(S)}} + \frac{1}{\omega - \varepsilon_k^{(S)}} \frac{|V_{Sd}|^2 P_{OO}^{dd}(\omega)}{X(\omega)} \frac{1}{\omega - \varepsilon_k^{(S)}} \right\} +$$

$$+ \sum_{k_1} \left\{ \frac{\delta_{kk_1}}{\omega - \epsilon_k^{(s)}} + \frac{1}{\omega - \epsilon_k^{(s)}} \frac{|V_{sd}|^2 P_{oo}^{dd}(\omega)}{\chi(\omega)} \frac{1}{\omega - \epsilon_{k_1}^{(s)}} \right\} Z_{k_1 k_1}^{ss}(\omega) +$$

$$+ \sum_{k_{1}} \left\{ \frac{1}{\omega - \varepsilon_{k}^{(s)}} \frac{v_{sd}}{x(\omega)} \frac{1}{\omega - \varepsilon_{k_{1}}^{(\omega)}} \right\} Z_{k_{1}k}^{ds} (\omega)$$
(19.c)

$$\Theta_{kk}^{ds}(\omega) = \sigma \langle S_{0}^{z} \rangle \left\{ \frac{1}{2\pi} \frac{1}{\omega - \varepsilon_{k}^{(s)}} \frac{V_{ds}}{X(\omega)} \frac{1}{\omega - \varepsilon_{k}^{(s)}} \right\} +$$

$$+ \sum_{k_{1}} \left\{ \frac{1}{\omega - \varepsilon_{k}^{(d)}} \frac{V_{ds}}{X(\omega)} \frac{1}{\omega - \varepsilon_{k_{1}}^{(s)}} \right\} Z_{k_{1}}^{ss} k'(\omega) +$$

$$+ \sum_{k_{1}} \left\{ \frac{\delta_{kk}}{\omega - \varepsilon_{k}^{(d)}} + \frac{1}{\omega - \varepsilon_{k}^{(d)}} \frac{V_{dd} + |V_{sd}|^{2} P_{oo}^{ss}(\omega)}{X(\omega)} \frac{1}{\omega - \varepsilon_{k_{1}}^{(d)}} \right\} Z_{k_{1}}^{ds} k'(\omega)$$

$$(19.f)$$

Using the results for the propagators G, one has:

$$\Theta_{kk}^{ss}(\omega) = \sigma < S_{0}^{z} > G_{kk}^{ss}(\omega) + 2\pi \sum_{k_{1}} G_{kk_{1}}^{ss}(\omega) Z_{k_{1}k}^{ss}(\omega) + 2\pi \sum_{k_{1}} G_{kk_{1}}^{sd}(\omega) Z_{k_{1}k}^{ds}(\omega)$$
(19.g)

$$\Theta_{kk}^{ds}(\omega) = \sigma < S_{0}^{z} > G_{kk}^{ds}(\omega) + 2\pi \sum_{k_{1}} G_{kk_{1}}^{ds}(\omega) Z_{k_{1}k}^{ss}(\omega) + 2\pi \sum_{k_{1}} G_{kk_{1}}^{dd}(\omega) Z_{k_{1}k}^{ds}(\omega)$$
(19.h)

Finally, in the Wannier representation:

$$\Theta_{\mathbf{i}\,\mathbf{j}}^{SS}(\omega) = \sigma \langle S_{\mathbf{o}}^{Z} \rangle G_{\mathbf{i}\,\mathbf{j}}^{SS}(\omega) + 2\pi \sum_{m} G_{\mathbf{i}\,m}^{SS}(\omega) Z_{m\mathbf{j}}^{SS}(\omega) + 2\pi \sum_{m} G_{\mathbf{i}\,m}^{S\,\mathbf{d}}(\omega) Z_{m\mathbf{j}}^{\mathbf{d}s}(\omega)$$
 (20.a)

$$\Theta_{i,j}^{ds}(\omega) = \sigma \langle S_{o}^{z} \rangle G_{i,j}^{ds}(\omega) + 2\pi \sum_{m} G_{i,m}^{ds}(\omega) Z_{m,j}^{ss}(\omega) + 2\pi \sum_{m} G_{i,m}^{dd}(\omega) Z_{m,j}^{ds}(\omega)$$
 (20.b)

It remains to collect terms involved in the functions  $Z_{mj}$ . Equations (19.c) and (19.d) can be rewritten as:

$$Z_{ij}^{ss}(\omega) = J^{(s)} \left\{ S_{0}(S_{0} + 1) \delta_{i0} - 3\beta_{i0}^{ss} \right\} \Gamma_{0j}^{ss}(\omega) - J^{(s)} \left\{ \delta_{i0} - 2\alpha_{i0}^{ss} \right\} \Theta_{0j}^{ss}(\omega) + 2 J^{(d)} \alpha_{i0}^{sd} \Theta_{0j}^{ds}(\omega) - 3 J^{(d)} \beta_{i0}^{sd} \Gamma_{0j}^{ds}(\omega)$$
(20.c)

and

$$Z_{ij}^{ds}(\omega) = 2 J^{(s)} \alpha_{io}^{ds} \Theta_{oj}^{ss}(\omega) - 3 J^{(s)} \beta_{io}^{ds} \Gamma_{oj}^{ss}(\omega) +$$

$$+ J^{(d)} \left\{ S_{o}(S_{o} + 1) \delta_{io} - 3 \beta_{io}^{dd} \right\} \Gamma_{oj}^{ds}(\omega) -$$

$$- J^{(d)} \left\{ \delta_{io} - 2 \alpha_{io}^{dd} \right\} \Theta_{oj}^{ds}(\omega)$$
(20.d)

At this point it is useful to introduce a matrix notation.

#### (c.iii) INTEGRAL EQUATION IN MATRIX FORM

Using the matrices  $A^{\alpha\beta}(\omega)$  and  $D^{\alpha\beta}(\omega)$ ,  $(\alpha, \beta = s,d)$  defined in Appendix B, equations (20) become:

$$\hat{D}^{SS}(\omega) \cdot \hat{\Theta}^{SS}(\omega) = \sigma \langle S_0^z \rangle \hat{G}^{SS}(\omega) + \hat{A}^{SS}(\omega) \cdot \hat{\Gamma}^{SS}(\omega) + \hat{A}^{Sd}(\omega) \cdot \hat{\Gamma}^{dS}(\omega) + \hat{D}^{Sd}(\omega) \cdot \hat{\Theta}^{dS}(\omega)$$
(21.a)

$$\hat{D}^{\mathrm{dd}}(\omega) \cdot \hat{\Theta}^{\mathrm{ds}}(\omega) = \sigma \langle S_{0}^{z} \rangle \hat{G}^{\mathrm{ds}}(\omega) + \hat{A}^{\mathrm{dd}}(\omega) \cdot \hat{\Gamma}^{\mathrm{ds}}(\omega) + \hat{A}^{\mathrm{ds}}(\omega) \cdot \hat{\Gamma}^{\mathrm{ss}}(\omega) + \hat{D}^{\mathrm{ds}}(\omega) \cdot \hat{\Theta}^{\mathrm{ss}}(\omega)$$
(21.b)

Quite similarly, introducing the  $\gamma_{\beta}^{\alpha\beta}(\omega)$  matrix, defined by:

$$\left\{\gamma_{\beta}^{\alpha\beta}(\omega)\right\}_{ij} = 2\pi J^{(\beta)} G_{io}^{\alpha\beta}(\omega) \delta_{oj} \qquad (\alpha, \beta = s,d) \quad (21.c)$$

equations (18) can be rewritten as:

$$\widehat{T}^{SS}(\omega) = \widehat{G}^{SS}(\omega) + \widehat{\gamma}_{S}^{SS}(\omega) \cdot \widehat{\Theta}^{SS}(\omega) + \widehat{\gamma}_{d}^{Sd}(\omega) \cdot \widehat{\Theta}^{dS}(\omega)$$
 (21.d)

$$\hat{\Gamma}^{ds}(\omega) = \hat{G}^{ds}(\omega) + \hat{\gamma}_{d}^{dd}(\omega) \cdot \hat{\Theta}^{ds}(\omega) + \hat{\gamma}_{s}^{ds}(\omega) \cdot \hat{\Theta}^{ss}(\omega)$$
 (21.e)

The set of coupled matrix equations (21.a), (21.b), (21.d) and (21.e) completely specify the involved propagators in terms of the G's. In order

to obtain an integral equation for the  $\hat{\Gamma}^{SS}(\omega)$  propagator, we start eliminating in (20.a) and (20.b) the propagator  $\hat{\Gamma}^{dS}(\omega)$  using equation (21.e); one gets:

$$\hat{\Delta}^{SS}(\omega) \cdot \hat{\Theta}^{SS}(\omega) = \sigma \langle S_0^z \rangle \hat{G}^{SS}(\omega) + \hat{A}^{Sd}(\omega) \cdot \hat{G}^{dS}(\omega) + \hat{A}^{SS}(\omega) \cdot \hat{\Gamma}^{SS}(\omega) + \hat{\Delta}^{Sd}(\omega) \cdot \hat{\Theta}^{dS}(\omega)$$
(22.a)

$$\hat{\Delta}^{\mathrm{dd}}(\omega) \cdot \hat{\Theta}^{\mathrm{ds}}(\omega) = \sigma < S_{\hat{O}}^{\mathsf{Z}} > \hat{\mathsf{G}}^{\mathrm{ds}}(\omega) + \hat{\mathsf{A}}^{\mathrm{dd}}(\omega) \cdot \hat{\mathsf{G}}^{\mathrm{ds}}(\omega) + \hat{\mathsf{A}}^{\mathrm{ds}}(\omega) \cdot \hat{\mathsf{G}}^{\mathrm{ss}}(\omega) + \hat{\Delta}^{\mathrm{ds}}(\omega) \cdot \hat{\Theta}^{\mathrm{ss}}(\omega)$$
(22.b)

where we have defined:

$$\hat{\Delta}^{ss}(\omega) = \hat{D}^{ss}(\omega) - \hat{A}^{sd}(\omega) \cdot \hat{\gamma}_{s}^{ds}(\omega)$$

$$\hat{\Delta}^{dd}(\omega) = \hat{D}^{dd}(\omega) - \hat{A}^{dd}(\omega) \cdot \hat{\gamma}_{d}^{dd}(\omega)$$

$$\hat{\Delta}^{sd}(\omega) = \hat{D}^{sd}(\omega) + \hat{A}^{sd}(\omega) \cdot \hat{\gamma}_{d}^{dd}(\omega)$$

$$\hat{\Delta}^{ds}(\omega) = \hat{D}^{ds}(\omega) + \hat{A}^{dd}(\omega) \cdot \hat{\gamma}_{s}^{ds}(\omega)$$

$$(22.c)$$

From equations (22) we are able to get explicit expressions for  $\hat{\Theta}^{SS}(\omega)$  and  $\hat{\Theta}^{dS}(\omega)$  in terms of  $\hat{\Gamma}^{SS}(\omega)$ .

Introducing the matrix  $M^{SS}(\omega)$  as:

$$\widehat{M}^{SS}(\omega) = \widehat{\mathbf{I}} - (\widehat{\Delta}^{SS}(\omega))^{-1} \cdot \widehat{\Delta}^{Sd}(\omega) \cdot (\widehat{\Delta}^{dd}(\omega))^{-1} \widehat{\Delta}^{ds}(\omega)$$

one gets:

$$\begin{split} \widehat{\Theta}^{SS}(\omega) = & \sigma \langle S_{O}^{Z} \rangle (\widehat{\Delta}^{SS}(\omega) \cdot \widehat{M}^{SS}(\omega))^{-1} \cdot \left[ \widehat{G}^{SS}(\omega) + \widehat{\Delta}^{Sd}(\omega) \cdot (\widehat{\Delta}^{dd}(\omega))^{-1} \cdot \widehat{G}^{dS}(\omega) \right] \\ & + (\widehat{\Delta}^{SS}(\omega) \cdot \widehat{M}^{SS}(\omega))^{-1} \cdot \left[ \widehat{A}^{Sd}(\omega) + \widehat{\Delta}^{Sd}(\omega) \cdot (\widehat{\Delta}^{dd}(\omega))^{-1} \cdot \widehat{A}^{dd}(\omega) \right] \cdot \widehat{G}^{dS}(\omega) \\ & + (\widehat{\Delta}^{SS}(\omega) \cdot \widehat{M}^{SS}(\omega))^{-1} \cdot \left[ \widehat{A}^{SS}(\omega) + \widehat{\Delta}^{Sd}(\omega) \cdot (\widehat{\Delta}^{dd}(\omega))^{-1} \cdot \widehat{A}^{dS}(\omega) \right] \cdot \widehat{\Gamma}^{SS}(\omega) \end{split}$$

and:

$$\begin{split} \widehat{\Theta}^{ds}(\omega) = & \sigma < S_{0}^{z} > (\widehat{\Delta}^{dd}(\omega))^{-1} \cdot \left\{ \left[ \widehat{1} + \widehat{\Delta}^{ds}(\omega) \cdot (\widehat{\Delta}^{ss}(\omega) \cdot \widehat{M}^{ss}(\omega))^{-1} \cdot \widehat{\Delta}^{sd}(\omega) \cdot (\widehat{\Delta}^{dd}(\omega))^{-1} \right] \cdot \widehat{G}^{ss}(\omega) + \\ & + \widehat{\Delta}^{ds}(\omega) \cdot (\widehat{\Delta}^{ss}(\omega) \cdot \widehat{M}^{ss}(\omega))^{-1} \cdot \widehat{G}^{ss}(\omega) \right\} + \\ & + (\widehat{\Delta}^{dd}(\omega))^{-1} \cdot \left\{ \widehat{A}^{dd}(\omega) + \widehat{\Delta}^{ds}(\omega) \cdot (\widehat{\Delta}^{ss}(\omega) \cdot \widehat{M}^{ss}(\omega))^{-1} \cdot \left[ \widehat{A}^{sd}(\omega) + \right. \right. \\ & + \left. \left( \widehat{\Delta}^{dd}(\omega) \right)^{-1} \cdot \widehat{A}^{dd}(\omega) \right] \right\} \cdot \widehat{G}^{ds}(\omega) + \\ & + (\widehat{\Delta}^{dd}(\omega))^{-1} \cdot \left\{ \widehat{A}^{ds}(\omega) + \widehat{\Delta}^{ds}(\omega) \cdot (\widehat{\Delta}^{ss}(\omega) \cdot \widehat{M}^{ss}(\omega))^{-1} \cdot \left[ \widehat{A}^{ss}(\omega) + \right. \right. \\ & + \left. \left( \widehat{\Delta}^{sd}(\omega) \right)^{-1} \cdot \widehat{A}^{ds}(\omega) \right\} \right\} \cdot \widehat{T}^{ss}(\omega) \end{split}$$

Equations (23.a) and (23.b) substituted into (21.d) provide the final form of the integral equation for  $\hat{\Gamma}^{SS}(\omega)$ .

Let us introduce the following auxiliary definitions: (self-energies)

$$\hat{\Sigma}_{(1)}^{sd}(\omega) = \hat{\gamma}_{s}^{ss}(\omega) \cdot (\hat{\Delta}^{ss}(\omega) \cdot \hat{H}^{ss}(\omega))^{-1} \cdot \left[ \hat{A}^{sd}(\omega) + \hat{\Delta}^{sd}(\omega) \cdot (\hat{\Delta}^{dd}(\omega))^{-1} \cdot \hat{A}^{dd}(\omega) \right] + \\
+ \hat{\gamma}_{d}^{sd}(\omega) \cdot (\hat{\Delta}^{dd}(\omega))^{-1} \cdot \left[ \hat{A}^{dd}(\omega) + \hat{\Delta}^{ds}(\omega) \cdot (\hat{\Delta}^{ss}(\omega) \cdot \hat{M}^{ss}(\omega))^{-1} \cdot \left[ \hat{A}^{sd}(\omega) + \hat{\Delta}^{sd}(\omega) + \hat{\Delta}^{sd}(\omega) \cdot (\hat{\Delta}^{ss}(\omega) \cdot \hat{M}^{ss}(\omega))^{-1} \cdot \hat{A}^{sd}(\omega) + \hat{\Delta}^{sd}(\omega) \cdot (\hat{\Delta}^{sd}(\omega))^{-1} \cdot \hat{A}^{sd}(\omega) \right] + \\
+ \hat{\Delta}^{sd}(\omega) \cdot (\hat{\Delta}^{dd}(\omega))^{-1} \cdot \hat{A}^{dd}(\omega) \Big] \right\}$$
(24.a)

$$\hat{\sum}_{(1)}^{SS}(\omega) = \hat{\gamma}_{S}^{SS}(\omega) \cdot (\hat{\Delta}^{SS}(\omega) \cdot \hat{M}^{SS}(\omega))^{-1} \cdot \left[ \hat{A}^{SS}(\omega) + \hat{\Delta}^{Sd}(\omega) \cdot (\hat{\Delta}^{dd}(\omega))^{-1} \cdot \hat{A}^{dS}(\omega) \right] +$$

$$\hat{\gamma}_{d}^{Sd}(\omega) \cdot (\hat{\Delta}^{dd}(\omega))^{-1} \cdot \left\{ \hat{A}^{dS}(\omega) + \hat{\Delta}^{dS}(\omega) \cdot (\hat{\Delta}^{SS}(\omega) \cdot \hat{M}^{SS}(\omega))^{-1} \cdot \left[ \hat{A}^{SS}(\omega) + \hat{\Delta}^{SS}(\omega) + \hat{\Delta}^{SS}(\omega) \right] \right\} +$$

$$+ \hat{\Delta}^{Sd}(\omega) \cdot (\hat{\Delta}^{dd}(\omega))^{-1} \cdot \hat{A}^{dS}(\omega) \right\}$$

$$(24.b)$$

The terms proportional to  $\langle S^z \rangle$  contribute the self-energies:

$$\hat{\sum}_{(2)}^{SS}(\omega) = \hat{\gamma}_{S}^{SS}(\omega) \cdot (\hat{\triangle}^{SS}(\omega) \cdot \hat{M}^{SS}(\omega))^{-1} + \hat{\gamma}_{d}^{Sd}(\omega) \cdot (\hat{\triangle}^{dd}(\omega))^{-1} \cdot \hat{\triangle}^{dS}(\omega) \cdot (\hat{\triangle}^{SS}(\omega) \cdot \hat{M}^{SS}(\omega))^{-1}$$
and finally.

(24.c)

and finally:

$$\widehat{\Sigma}_{(2)}^{sd}(\omega) = \widehat{\gamma}_{s}^{ss}(\omega) \cdot (\widehat{\Delta}^{ss}(\omega) \cdot \widehat{M}^{ss}(\omega))^{-1} \cdot \widehat{\Delta}^{sd}(\omega) \cdot (\widehat{\Delta}^{dd}(\omega))^{-1} + \\
+ \widehat{\gamma}_{d}^{sd}(\omega) \cdot (\widehat{\Delta}^{dd}(\omega))^{-1} \cdot \widehat{\Gamma}_{1} + \widehat{\Delta}^{ds}(\omega) \cdot (\widehat{\Delta}^{ss}(\omega) \cdot \widehat{M}^{ss}(\omega))^{-1} \cdot \widehat{\Delta}^{sd}(\omega) \cdot (\widehat{\Delta}^{dd}(\omega))^{-1} \right]$$
(24. d)

Using these definitions, the final result for the integral equation defining  $\widehat{\Gamma}^{SS}(\omega)$  is:

$$\widehat{\Gamma}^{SS}(\omega) = \widehat{G}^{SS}(\omega) + \sigma \langle S_0^z \rangle \widehat{\Sigma}_{(2)}^{SS}(\omega) \cdot \widehat{G}^{SS}(\omega) + \sigma \langle S_0^z \rangle \widehat{\Sigma}_{(2)}^{Sd}(\omega) \cdot \widehat{G}^{dS}(\omega) +$$

$$+ \widehat{\Sigma}_{(1)}^{Sd}(\omega) \cdot \widehat{G}^{dS}(\omega) + \widehat{\Sigma}_{(1)}^{SS}(\omega) \cdot \widehat{\Gamma}^{SS}(\omega)$$
(25)

#### III. TEMPERATURE INDEPENDENT RESISTIVITY

a) SECOND ORDER SOLUTION OF EQUATION (25)

In the absence of magnetic order, one has:

$$\langle S_0^z \rangle = 0$$

In this case one just needs  $\hat{\sum}_{(1)}^{SS}(\omega)$  and  $\hat{\sum}_{(1)}^{Sd}(\omega)$ . From expressions (22.c):

$$\Delta_{ij}^{ss}(\omega) = \delta_{ij} + O(J)$$

$$\Delta_{ij}^{dd}(\omega) = \delta_{ij} + O(J)$$

$$\Delta_{ij}^{sd}(\omega) = \delta_{ij} + O(J)$$

$$\Delta_{ij}^{ds}(\omega) = \delta_{ij} + O(J)$$

$$\Delta_{ij}^{ds}(\omega) = \delta_{ij} + O(J)$$
(26.a)

Using definitions (A-1) - see Appendix A - it follows that:

$$A_{ij}^{SS}(\omega) = 2\pi S_{o}(S_{o}+1) J^{(S)} G_{io}^{SS}(\omega) \delta_{jo} + O(J^{2})$$

$$A_{ij}^{dd}(\omega) = 2\pi S_{o}(S_{o}+1) J^{(d)} G_{io}^{dd}(\omega) \delta_{jo} + O(J^{2})$$

$$A_{ij}^{ds}(\omega) = 2\pi S_{o}(S_{o}+1) J^{(S)} G_{io}^{ds}(\omega) \delta_{jo} + O(J^{2})$$

$$A_{ij}^{Sd}(\omega) = 2\pi S_{o}(S_{o}+1) J^{(d)} G_{io}^{Sd}(\omega) \delta_{jo} + O(J^{2})$$

$$A_{ij}^{Sd}(\omega) = 2\pi S_{o}(S_{o}+1) J^{(d)} G_{io}^{Sd}(\omega) \delta_{jo} + O(J^{2})$$

Relations (26.a), (26.b) imply:

$$\hat{\Delta}^{\text{dd}}(\omega) \hat{j}_{ij}^{-1} = \delta_{ij} + O(J)$$

$$\hat{\Delta}^{\text{SS}}(\omega) \cdot \hat{M}^{\text{SS}}(\omega) \hat{j}_{ij}^{-1} = \delta_{ij} + O(J)$$

$$\hat{\Delta}^{\text{Sd}}(\omega) \cdot (\hat{\Delta}^{\text{dd}}(\omega))^{-1} \cdot \hat{A}^{\text{ds}}(\omega) \hat{j}_{ij} = O(J^{2})$$

$$\hat{\Delta}^{\text{Sd}}(\omega) \cdot (\hat{\Delta}^{\text{dd}}(\omega))^{-1} \cdot \hat{A}^{\text{dd}}(\omega) \hat{j}_{ij} = O(J^{2})$$

These results give the approximated (to second order in J) self-energies:

$$\sum_{(i)}^{ss} (\omega) \cong \hat{\gamma}_{s}^{ss} (\omega) \cdot \hat{A}^{ss} (\omega) + \hat{\gamma}_{d}^{sd} (\omega) \hat{A}^{ds} (\omega)$$
 (27.a)

$$\hat{\sum}_{(1)}^{sd}(\omega) \cong \hat{\gamma}_{s}^{ss}(\omega) \cdot \hat{A}^{sd}(\omega) + \hat{\gamma}_{d}^{sd}(\omega) \cdot \hat{A}^{dd}(\omega)$$
 (27.b)

Thus, the  $\hat{\Gamma}^{SS}(\omega)$  propagator reads:

$$\hat{\Gamma}^{SS}(\omega) = \hat{G}^{SS}(\omega) + \hat{\gamma}_{S}^{SS}(\omega) \cdot \hat{A}^{SS}(\omega) \cdot \hat{G}^{SS}(\omega) + \hat{\gamma}_{d}^{SS}(\omega) \cdot \hat{A}^{dS}(\omega) \cdot \hat{G}^{dS}(\omega) + + + \hat{\gamma}_{S}^{SS}(\omega) \cdot \hat{A}^{Sd}(\omega) \cdot \hat{G}^{dS}(\omega) + \hat{\gamma}_{d}^{Sd}(\omega) \cdot \hat{A}^{dd}(\omega) \cdot \hat{G}^{dS}(\omega)$$

$$(28)$$

or, in the Wannier representation (by using equations (21.C) and (26.b)):

$$\Gamma_{ij}^{ss}(\omega) = G_{ij}^{ss}(\omega) + (2\pi)^{2} S_{o}(S_{o}^{+1}) G_{io}^{ss}(\omega) J^{(s)} G_{oo}^{ss}(\omega) J^{(s)} G_{oj}^{ss}(\omega) +$$

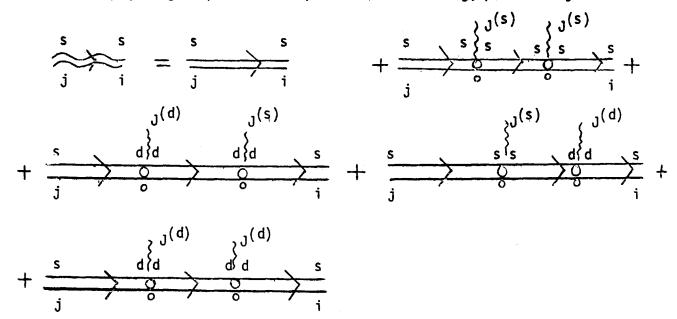
$$+ (2\pi)^{2} S_{o}(S_{o}^{+1}) G_{io}^{sd}(\omega) J^{(d)} G_{oo}^{ds}(\omega) J^{(s)} G_{oj}^{ss}(\omega) +$$

$$+ (2\pi)^{2} S_{o}(S_{o}^{+1}) G_{io}^{ss}(\omega) J^{(s)} G_{oo}^{sd}(\omega) J^{(d)} G_{oj}^{ds}(\omega) +$$

$$+ (2\pi)^{2} S_{o}(S_{o}^{+1}) G_{io}^{sd}(\omega) J^{(d)} G_{oo}^{dd}(\omega) J^{(d)} G_{oj}^{ds}(\omega) .$$

$$(29)$$

Equation (29) describes the four possible scattering processes involving electrons propagating in presence of potential scattering; pictorially:



Making use of the explicit expressions relating G-matrices and pure host propagators P, (see equations (8), (9), (10), (16.c)), one finds the final result:

$$\Gamma_{ij}^{SS}(\omega) = \frac{1}{2\pi} P_{ij}^{SS}(\omega) + \frac{1}{2\pi} P_{io}^{SS}(\omega) T(\omega) P_{oj}^{SS}(\omega)$$
 (30.a)

where:

$$T(\omega) = \frac{|V_{sd}|^2 P_{00}^{dd}(\omega)}{X(\omega)} +$$

$$+ \frac{S_{o}(S_{o}+1)\{(J^{(s)})^{2}(1-V_{dd}P_{oo}^{dd}(\omega))^{3}P_{oo}^{SS}(\omega)+2|V_{sd}|^{2}J^{(s)}J^{(d)}P_{oo}^{SS}(\omega)(P_{oo}^{dd}(\omega))^{2}(1-V_{dd}P_{oo}^{dd}(\omega))+(J^{(d)})^{2}|V_{sd}|^{2}P_{oo}^{dd}(\omega))^{3}}{(X(\omega))^{3}}$$
(30.b)

Remembering definition (6.c), one has:

$$P_{00}^{\lambda\lambda}(\omega) = \sum_{k} \frac{1}{\omega - \varepsilon_{k}(\lambda)} = F_{\lambda}(\omega), \qquad \lambda = s, d$$
 (30.c)

Hence, the T-matrix assumes this version:

$$i(\omega) = \frac{|V_{sd}|^2 F_d(\omega)}{X(\omega)} +$$

$$+ \frac{S_{0}(S_{0}+1)\{(J^{(s)})^{2}(1-V_{dd}F_{d}(\omega))^{3}F_{s}(\omega)+2|V_{sd}|^{2}J^{(s)}J^{(d)}F_{s}(\omega)(F_{d}(\omega))^{2}(1-V_{dd}F_{d}(\omega))+(J^{(d)})^{2}|V_{sd}|^{2}(F_{d}(\omega))^{3}\}}{(X(\omega))^{3}}$$

$$(X(\omega))^{3}$$

$$(30.d)$$

#### b) CALCULATION OF THE RESISTIVITY

In order to calculate the resistivity, one needs firstly to obtain an expression for  $ImT(\omega)$ . Introducing the concept of phase - shift <sup>7</sup>, one writes:

$$F_s(\omega) = F_s(\omega) e^{-i\delta_s(\omega)}$$

$$F_{d}(\omega) = |F_{d}(\omega)| e^{-i\delta_{d}(\omega)}$$

$$1 - V_{dd} F_{d}(\omega) = |1 - V_{dd} F_{d}(\omega)| e^{-i \eta_{dd}(\omega)} = |K(\omega)| e^{-i \eta_{dd}(\omega)}$$
(31)

$$X(\omega) = |X(\omega)| e^{-i\eta(\omega)}$$

where  $|F_S(\omega)|$ ,  $|F_d(\omega)|$ ,  $|K(\omega)|$ ,  $|X(\omega)|$   $\delta_S(\omega)$ ,  $\delta_d(\omega)$ ,  $n_{dd}(\omega)$  and  $n(\omega)$  are defined in Appendix B.

Substituting (31) into (30.d), one gets:

$$T(\omega) = |V_{sd}|^2 \frac{|F_d(\omega)|}{|X(\omega)|} e^{-i \left[\delta_d(\omega) - \eta(\omega)\right]_+}$$

$$+ S_{0}(S_{0}+1) \left\{ (J^{(S)})^{2} \frac{|K(\omega)|^{3}}{|X(\omega)|^{3}} |F_{S}(\omega)| e^{-i\left[3(\eta_{dd}(\omega)-\eta(\omega))+\delta_{S}(\omega)\right]} + \right.$$

$$+2|V_{sd}|^2J^{(s)}J^{(d)} = \frac{|K(\omega)||F_{s}(\omega)||F_{d}(\omega)|^2}{|X(\omega)|^3} e^{-i\left[n_{dd}(\omega)+\delta_{s}(\omega)+2\delta_{d}(\omega)-3n(\omega)\right]} +$$

$$d^{2} \left(J^{(d)}\right)^{2} \frac{|F_{d}(\omega)|^{3}}{|X(\omega)|^{3}} e^{-3i\left[\delta_{d}(\omega)-\eta(\omega)\right]}$$

$$(32)$$

Im 
$$T(\omega) = -|V_{sd}|^2 \frac{|F_d(\omega)|}{|X(\omega)|} \sin \left[\delta_d(\omega) - \eta(\omega)\right] -$$

$$-S_{o}(S_{o}+1)\left\{ (J^{(s)})^{2} \frac{|K(\omega)|^{3}}{|X(\omega)|^{3}} |F_{s}(\omega)| \sin\left[3(\eta_{dd}(\omega)-\eta(\omega)) + \delta_{s}(\omega)\right] + \right\}$$

$$+2|V_{sd}|^2 J^{(s)}J^{(d)} \frac{|K(\omega)||F_s(\omega||F_d(\omega)|^2}{|X(\omega)|^3} \sin \left[ n_{dd}(\omega) + \delta_s(\omega) + 2\delta_d(\omega) - 3n(\omega) \right] +$$

$$+ |V_{sd}|^{2} (J^{(d)})^{2} \frac{|F_{d}(\omega)|^{s}}{|X(\omega)|^{s}} \sin \left[3(\delta_{d}(\omega) - \eta(\omega))\right]$$
(33)

Consider a small concentration c of randomly distributed impurities. The effective life-time due to the impurities is:

$$\frac{h}{\tau_k} = -c \operatorname{Im} T(\omega) \tag{34}$$

If the electric conductivity per unit volume can be represented by a scalar (e.g. for crystals of cubic symmetry), one has:

$$\sigma = \frac{e^2}{12\pi^3 \, \text{fi}} \int \tau_k \, v_k^2 \left( -\frac{\partial f}{\partial \epsilon_k} \right) \, d^3k \qquad (35.a)$$

where f is the Fermi-Dirac distribution function and  $v_k$  is the electron group velocity. Transforming the integral over a volume of k space into integrations over constant energy surfaces (35.a) simplifies to:

$$\sigma = \frac{e^2 \tau_F}{12 \pi^3 f_0} \int v_F^2 dS_F$$
 (35.b)

(The subscript F indicates that the calculation is performed at the Fermi surface).

The resistivity is:

$$r = A \frac{\pi}{\tau_{F}}$$
 (36.a)

where:

$$A = \frac{3\Omega}{e^2 v_F^2 \rho_S(\varepsilon_F)}$$
 (36.b)

 $\Omega$  being the atomic volume and  $\rho$  the density of states. (Isotropic Fermi surface). From the above results, one finds for the temperature independent resistivity:

$$r = Ac|V_{sd}|^2 \frac{|F_d(\varepsilon_F)|}{|X(\varepsilon_F)|} \sin \left[\delta_d(\varepsilon_F) - \eta(\varepsilon_F)\right] +$$

+ Ac S<sub>0</sub>(S<sub>0</sub>+1) 
$$\left\{ (J^{(s)})^2 \frac{|K(\epsilon_F)|^3}{|X(\epsilon_F)|^3} |F_s(\epsilon_F)| \sin \left[ 3(\eta_{dd}(\epsilon_F) \eta(\epsilon_F)) + \delta_s(\epsilon_F) \right] + \right.$$

$$+2|V_{sd}|^2J^{(s)}J^{(d)} \frac{|K(\epsilon_F)||F_s(\epsilon_F)||F_d(\epsilon_F)|^2}{|X(\epsilon_F)|^3} sin \left[n_{dd}(\epsilon_F)+\delta_s(\epsilon_F)+2\delta_d(\epsilon_F)-3n(\epsilon_F)\right]+$$

$$+ |V_{sd}|^{2} (J^{(d)})^{2} \frac{|F_{d}(\varepsilon_{F})|^{3}}{|X(\varepsilon_{F})|^{3}} \sin \left[3(\delta_{d}(\varepsilon_{F}) - \eta(\varepsilon_{F}))\right]$$
(37)

Equation (37) may be written in a more convenient form. Denoting the exchange independent term  $Ac|V_{sd}|^2 \left\{ \frac{|F_d(\epsilon_F)|}{|X(\epsilon_F)|} \sin\left[\delta_d(\epsilon_F) - \eta(\epsilon_F)\right] \right\}$  by  $\Delta r_o(\epsilon_F)$ , and remembering that (cf. Appendix B):

$$|F_{s}(\varepsilon_{F})| \sin \delta_{s}(\varepsilon_{F}) = F_{s}^{I}(\varepsilon_{F}) = \pi \rho_{s}(\varepsilon_{F})$$
  
 $|F_{s}(\varepsilon_{F})| \cos \delta_{s}(\varepsilon_{F}) = F_{s}^{R}(\varepsilon_{F})$ 

it follows:

$$r = \Delta r_0(\varepsilon_F) + \pi \operatorname{Ac} S_0(S_0+1)(J^{(s)})^2 \rho_s(\varepsilon_F) \left\{ 1 + H(\varepsilon_F, |V_{sd}|^2) \right\}$$
 (38)

where:

$$H(\varepsilon_{F}, |V_{sd}|^{2}) = \frac{|K(\varepsilon_{F})|^{3}}{|X(\varepsilon_{F})|^{3}} \cos \left[3(n_{dd}(\varepsilon_{F}) - n(\varepsilon_{F}))\right] +$$

$$+\frac{|K(\varepsilon_{F})|^{3}}{|X(\varepsilon_{F})|^{3}}\frac{F_{s}^{R}(\varepsilon_{F})}{\pi \rho_{s}(\varepsilon_{F})}\sin \left[3(\eta_{dd}(\varepsilon_{F})-\eta(\varepsilon_{F})\right]+$$

$$+2|V_{sd}|^{2}\frac{J^{(d)}}{J^{(s)}}\frac{1}{\pi\rho_{s}(\varepsilon_{F})}\frac{|K(\varepsilon_{F})||F_{s}(\varepsilon_{F})||F_{d}(\varepsilon_{F})|^{2}}{|X(\varepsilon_{F})|^{2}}\sin\left[\eta_{dd}(\varepsilon_{F})+\right]$$

$$+ \delta_{s}(\epsilon_{F}) + 2\delta_{d}(\epsilon_{F}) - 3n(\epsilon_{F}) + |V_{sd}|^{2} \left(\frac{J(d)}{J(s)}\right)^{2} \frac{|F_{d}(\epsilon_{F})|^{3}}{|X(\epsilon_{F})|^{3}} \frac{1}{\pi \rho_{s}(\epsilon_{F})} \sin \left[3(\delta_{d}(\epsilon_{F}) - n(\epsilon_{F}))\right] - 1$$

Thus, it is possible to define an effective exchange coupling, namely:

$$J_{eff}^{(s)} = J^{(s)} \left[ 1 + H(\epsilon_F, |V_{sd}|^2) \right]^{1/2}$$
 (40)

and so:

$$r = \Delta r_0(\varepsilon_F) + \pi \operatorname{Ac} \rho_s(\varepsilon_F) (J_{eff}^{(s)})^2 S_0(S_0+1)$$
 (41)

In the absence of charge potential scattering, one has:

$$H(\varepsilon_F, |V_{sd}|^2) = 0 \implies J_{eff}^{(s)} = J^{(s)}$$

and the resistivity reduces to this simplified form:

$$r = \pi \text{ Ac } S_0(S_0+1) \left(J^{(S)}\right)^2 \rho_S(\varepsilon_F)$$
 (42)

#### **CONCLUSIONS**

As firstly discussed by Blackman and Elliott 4, a strong impurity potential (treated beyond the Born approximation) affects in a significant way the resistivity associated to a local moment. In their paper, however, the potential acting only in a single-band model, excludes the possibility of discussing transition metal-like hots. The latter systems suggest new possibilities of experimental work. In fact, the existence of two bands (s and d) and consequently two exchange couplings, may change the standard result of De Gennes and Friedel 8 as given by equation (42). This result has been extensively used (together with the Abrikosov-Gorkov picture of the decrease of superconductor temperature with concentration of magnetic rurities) as an experimental method for deriving coupling constants J. r, the result described in (38) shows that in the case of transition one may have strong deviations from the simple free electron case (42) n from the result obtained in ref. 4. In the former case  $^4$ , the fts associated to the spin independent impurity potential appear Ag only  $(J)^2$ .

In the transition metal case the situation is very different: one has phase-shifts multiplied by  $J^{(s)}$  and  $J^{(d)}$ , these exchange parameters appearing as  $(J^{(s)})^2$ ,  $(J^{(d)})^2$  and  $J^{(s)}$ . For suitable impurities (like Cerium)  $J^{(s)} < 0$ , so one has cross products which may strongly affect the magnitude of the derived  $J^{(s)}_{eff}$  (40). These results suggest that one should take into account, in the detailed comparison, of the calculated bare exchange parameters, the characteristic of the impurity with respect to the host. Expression (38) suggest also that, if rare-earth impurities are used, on may consider firstly Lu (no spin moment). In this case only the first term of (38) still remains. A resistivity measurement determines then the first term. When a  $S_0 \neq 0$  trivalent rare-earth impurity (e.g. Gd) is introduced in the same host, the first term of (38) is expected to remain nearly constant. In this way, one measures the contribution of the second term of (38).

Finally, we want to point out that the general equation (25) being valid to any order in perturbation theory, may serve as starting point for a calculation (similar to ref. 4) of the effect of the impurity potential in the logarithmic Kondo term.

#### APPENDIX A

DEFINITION OF THE MATRICES A( $\omega$ ) AND D( $\omega$ )

$$A_{ij}^{ss}(\omega) = 2\pi S_{o}(S_{o}+1)G_{io}^{ss}(\omega)J^{(s)}\delta_{jo} - 2\pi \sum_{m}J^{(s)}G_{im}^{ss}(\omega)3B_{mo}^{ss}\delta_{jo} - 2\pi \sum_{m}J^{(s)}G_{im}^{sd}(\omega)3B_{mo}^{ds}\delta_{jo} - 2\pi \sum_{m}J^{(s)}G_{im}^{sd}(\omega)3B_{mo}^{ds}\delta_{jo}$$
(A.1a)

$$A_{ij}^{dd}(\omega) = 2\pi S_{o}(S_{o}+1)G_{io}^{dd}(\omega)J^{(d)}\delta_{jo} - 2\pi \sum_{m}J^{(d)}G_{im}^{dd}(\omega)3\beta_{mo}^{dd}\delta_{jo} - 2\pi \sum_{m}J^{(d)}G_{im}^{ds}(\omega)3\beta_{mo}^{sd}\delta_{jo} - 2\pi \sum_{m}J^{(d)}G_{im}^{sd}(\omega)3\beta_{mo}^{sd}\delta_{jo} - 2\pi \sum_{m}J^{(d)}G_{im}^{sd}\delta_{jo} - 2\pi \sum_{m}J^{(d)}G_{im}^{sd}\delta_{j$$

$$A_{ij}^{sd}(\omega) = 2\pi S_{o}(S_{o}+1)G_{io}^{sd}(\omega)J^{(d)}\delta_{jo} - 2\pi \sum_{m}J^{(d)}G_{im}^{ss}(\omega)3\beta_{mo}^{sd}\delta_{jo} - 2\pi \sum_{m}J^{(d)}G_{im}^{sd}(\omega)3\beta_{mo}^{dd}\delta_{jo} - 2\pi \sum_{m}J^{(d)}G_{im}^{sd}(\omega)3\beta_{mo}^{sd}\delta_{jo} - 2\pi \sum_{m}J^{(d)}G_{im}^{sd}\delta_{jo} - 2\pi \sum_{m}J^{(d)}G_{im}^{sd}\delta_{j$$

$$A_{ij}^{ds}(\omega) = 2\pi S_{o}(S_{o}^{+1})G_{io}^{ds}(\omega)J^{(s)}\delta_{jo}^{-2\pi\sum_{m}J^{(s)}G_{im}^{dd}(\omega)3\beta_{mo}^{ds}\delta_{jo}^{-2\pi\sum_{m}J^{(s)}G_{im}^{ds}(\omega)3\beta_{mo}^{ss}\delta_{jo}^{-2\pi\sum_{m}J^{(s)}G_{im}^{ds}(\omega)3\beta_{mo}^{ss}\delta_{jo}^{-2\pi\sum_{m}J^{(s)}G_{im}^{ds}(\omega)3\beta_{mo}^{ss}\delta_{jo}^{-2\pi\sum_{m}J^{(s)}G_{im}^{ds}(\omega)3\beta_{mo}^{ss}\delta_{jo}^{-2\pi\sum_{m}J^{(s)}G_{im}^{ds}(\omega)3\beta_{mo}^{ss}\delta_{jo}^{-2\pi\sum_{m}J^{(s)}G_{im}^{ds}(\omega)3\beta_{mo}^{ss}\delta_{jo}^{-2\pi\sum_{m}J^{(s)}G_{im}^{ds}(\omega)3\beta_{mo}^{ss}\delta_{jo}^{-2\pi\sum_{m}J^{(s)}G_{im}^{ds}(\omega)3\beta_{mo}^{ss}\delta_{jo}^{-2\pi\sum_{m}J^{(s)}G_{im}^{ds}(\omega)3\beta_{mo}^{ss}\delta_{jo}^{-2\pi\sum_{m}J^{(s)}G_{im}^{ds}(\omega)3\beta_{mo}^{ss}\delta_{jo}^{-2\pi\sum_{m}J^{(s)}G_{im}^{ds}(\omega)3\beta_{mo}^{ss}\delta_{jo}^{-2\pi\sum_{m}J^{(s)}G_{im}^{ds}(\omega)3\beta_{mo}^{ss}\delta_{jo}^{-2\pi\sum_{m}J^{(s)}G_{im}^{ds}(\omega)3\beta_{mo}^{ss}\delta_{jo}^{-2\pi\sum_{m}J^{(s)}G_{im}^{ds}(\omega)3\beta_{mo}^{ss}\delta_{jo}^{-2\pi\sum_{m}J^{(s)}G_{im}^{ds}(\omega)3\beta_{mo}^{ss}\delta_{jo}^{-2\pi\sum_{m}J^{(s)}G_{im}^{ds}(\omega)3\beta_{mo}^{ss}\delta_{jo}^{-2\pi\sum_{m}J^{(s)}G_{im}^{ds}(\omega)3\beta_{mo}^{ss}\delta_{jo}^{-2\pi\sum_{m}J^{(s)}G_{im}^{ds}(\omega)3\beta_{mo}^{ss}\delta_{jo}^{-2\pi\sum_{m}J^{(s)}G_{im}^{ss}\delta_{jo}^{-2\pi\sum_{m}J^{(s)}G_{im}^{ss}\delta_{jo}^{-2\pi\sum_{m}J^{(s)}G_{im}^{ss}\delta_{jo}^{-2\pi\sum_{m}J^{(s)}G_{im}^{ss}\delta_{jo}^{-2\pi\sum_{m}J^{(s)}G_{im}^{ss}\delta_{jo}^{-2\pi\sum_{m}J^{(s)}G_{im}^{ss}\delta_{jo}^{-2\pi\sum_{m}J^{(s)}G_{im}^{ss}\delta_{jo}^{-2\pi\sum_{m}J^{(s)}G_{im}^{ss}\delta_{jo}^{-2\pi\sum_{m}J^{(s)}G_{im}^{ss}\delta_{jo}^{-2\pi\sum_{m}J^{(s)}G_{im}^{ss}\delta_{jo}^{-2\pi\sum_{m}J^{(s)}G_{im}^{ss}\delta_{jo}^{-2\pi\sum_{m}J^{(s)}G_{im}^{ss}\delta_{jo}^{-2\pi\sum_{m}J^{(s)}G_{im}^{ss}\delta_{jo}^{-2\pi\sum_{m}J^{(s)}G_{im}^{ss}\delta_{jo}^{-2\pi\sum_{m}J^{(s)}G_{im}^{ss}\delta_{jo}^{-2\pi\sum_{m}J^{(s)}G_{im}^{ss}\delta_{jo}^{-2\pi\sum_{m}J^{(s)}G_{im}^{ss}\delta_{jo}^{-2\pi\sum_{m}J^{(s)}G_{im}^{ss}\delta_{jo}^{-2\pi\sum_{m}J^{(s)}G_{im}^{ss}\delta_{jo}^{-2\pi\sum_{m}J^{(s)}G_{im}^{ss}\delta_{jo}^{-2\pi\sum_{m}J^{(s)}G_{im}^{ss}\delta_{jo}^{-2\pi\sum_{m}J^{(s)}G_{im}^{ss}\delta_{jo}^{-2\pi\sum_{m}J^{(s)}G_{im}^{ss}\delta_{jo}^{-2\pi\sum_{m}J^{(s)}G_{im}^{ss}\delta_{jo}^{-2\pi\sum_{m}J^{(s)}G_{im}^{ss}\delta_{jo}^{-2\pi\sum_{m}J^{(s)}G_{im}^{ss}\delta_{jo}^{-2\pi\sum_{m}J^{(s)}G_{im}^{ss}\delta_{jo}^{-2\pi\sum_{m}J^{(s)}G_{im}^{ss}\delta_{jo}^{-2\pi\sum_{m}J^{(s)}G_{im}^{ss}\delta_{jo}^{-2\pi\sum_{m}J^{(s)}G_{im}^{ss}\delta_{jo}^{-2\pi\sum_{m}J^{(s)}G_{im}^{ss}\delta$$

$$D_{ij}^{ss}(\omega) = \delta_{ij} + 2\pi G_{io}^{ss}(\omega) J^{(s)} \delta_{oj} - 2\pi \sum_{m} G_{im}^{ss}(\omega) 2\alpha_{mo}^{ss} J^{(s)} \delta_{oj} - 2\pi \sum_{m} G_{im}^{sd}(\omega) 2\alpha_{mo}^{ds} J^{(s)} \delta_{oj}$$
 (A.2a)

$$D_{ij}^{dd}(\omega) = \delta_{ij} + 2\pi G_{io}^{dd}(\omega) J^{(d)} \delta_{oj} - 2\pi \sum_{m} G_{im}^{dd}(\omega) 2\alpha_{mo}^{dd} J^{(d)} \delta_{oj} - 2\pi \sum_{m} G_{im}^{ds}(\omega) 2\alpha_{mo}^{sd} J^{(d)} \delta_{oj} \quad (A.2b)$$

$$D_{ij}^{sd}(\omega) = -2\pi G_{io}^{sd}(\omega) J^{(d)} \delta_{oj} + 2\pi \sum_{m} G_{im}^{ss}(\omega) 2\alpha_{mo}^{sd} J^{(d)} \delta_{oj} + 2\pi \sum_{m} G_{im}^{sd}(\omega) 2\alpha_{mo}^{dd} J^{(d)} \delta_{oj}$$
(A.2c)

$$D_{ij}^{ds}(\omega) = -2\pi G_{io}^{ds}(\omega) J^{(s)} \delta_{oj} + 2\pi \sum_{m} G_{im}^{dd}(\omega) 2\alpha_{mo}^{ds} J^{(s)} \delta_{oj} + 2\pi \sum_{m} G_{im}^{ds}(\omega) 2\alpha_{mo}^{ss} J^{(s)} \delta_{oj} \qquad (A.2d)$$

#### PHASE-SHIFT PARAMETERS

Taking into account definition (30.c), for  $\omega \pm i\delta$  in the limit  $\delta \to 0$ , one has real and imaginary parts. Hence:

$$F_{\lambda}(\omega + i\delta) = F_{\lambda}^{R}(\omega) + i F_{\lambda}^{I}(\omega)$$
,  $(\lambda = s,d)$  (B.1)

where:

$$F_{\lambda}^{R}(\omega) = P \sum_{k} \frac{1}{\omega - \varepsilon_{k}(\lambda)}; \quad F_{R}^{I}(\omega) = \pi \rho_{\lambda}(\omega)$$
 (B.2)

 $\rho_{\lambda}(\omega)$  denoting the density of states of conducting  $\lambda\text{-electrons.}$ 

If we introduce the "phase-shift", one may write:

$$F_{\lambda}(\omega + i\delta) = |F_{\lambda}(\omega)|e^{Fi\delta}\lambda^{(\omega)}$$
 (B.3)

where:

$$|F_{\lambda}(\omega)| = \left[ (F_{\lambda}^{R}(\omega))^{2} + (F_{\lambda}^{I}(\omega))^{2} \right]^{1/2}$$

$$\cos \delta_{\lambda}(\omega) = \frac{F_{\lambda}^{R}(\omega)}{|F_{\lambda}(\omega)|}$$
(B.4)

$$sin\delta_{\lambda}(\omega) = \frac{F_{\lambda}^{I}(\omega)}{|F_{\lambda}(\omega)|}$$

It is quite clear that:

$$F_{s}(\underline{\omega+i\delta})F_{d}(\underline{\omega+i\delta}) = |F_{s}(\underline{\omega})||F_{d}(\underline{\omega})| e^{\mp [i \delta_{s}(\underline{\omega})+\delta_{d}(\underline{\omega})]}$$
(B.5)

Similarly:

$$1-V_{dd}F_{d}(\omega\pm i\delta)=1-V_{dd}F_{d}^{R}(\omega)\pm i\ V_{dd}F_{d}^{I}(\omega)=|1-V_{dd}F_{d}(\omega)|\ e^{\mp i\ \eta_{dd}(\omega)} \tag{B.6}$$

where:

$$|1-V_{dd}F_{d}(\omega)| = [(1-V_{dd}F_{d}^{R}(\omega))^{2} + (V_{dd}F_{d}^{I}(\omega))^{2}]^{1/2}$$

$$\cos n_{dd}(\omega) = \frac{1 - V_{dd} F_d^R(\omega)}{1 - V_{dd} F_d(\omega)}$$
(B.7)

$$\sin \eta_{dd}(\omega) = -\frac{V_{dd} F_{d}^{I}(\omega)}{|1-V_{dd} F_{d}(\omega)|}$$

and finally:

$$1-V_{dd} F_{d}(\omega \pm i\delta) - |V_{sd}|^2 F_{s}(\omega \pm i\delta) F_{d}(\omega \pm i\delta) = |X(\omega)| e^{\mp i\eta(\omega)}$$
(B.8)

whe re

$$|X(\omega)| = \{ [1 - V_{dd}F_{d}^{R}(\omega) - |V_{sd}|^{2} (F_{d}^{R}(\omega)F_{s}^{R}(\omega) - F_{d}^{I}(\omega)F_{s}^{I}(\omega)) ]^{2} + [V_{dd}F_{d}^{I}(\omega) - |V_{sd}|^{2} (F_{d}^{R}(\omega)F_{s}^{I}(\omega) + F_{d}^{I}(\omega)F_{s}^{R}(\omega)) ]^{2} \}^{1/2}$$

$$\cos \eta(\omega) = \frac{1 - V_{dd} F_d^R(\omega) - |V_{sd}|^2 (F_d^R(\omega) F_s^R(\omega) - F_d^I(\omega) F_s^I(\omega))}{|X(\omega)|}$$
(B.9)

$$\sin \eta(\omega) = -\frac{V_{dd} F_d^I(\omega) - |V_{sd}|^2 (F_d^R(\omega) F_s^I(\omega) + F_d^I(\omega) F_s^R(\omega))}{|X(\omega)|}$$

#### APPENDIX C

The spin independent contribution to the resistivity is:

$$\Delta r_{o} = Ac |V_{sd}|^{2} \frac{|F_{d}(\varepsilon_{F})|}{|X(\varepsilon_{F})|} \{ \sin \delta_{d}(\varepsilon_{F}) \cos \eta(\varepsilon_{F}) - \cos \delta_{d}(\varepsilon_{F}) \sin \eta(\varepsilon_{F}) \}$$

$$= \frac{Ac|V_{sd}|^{2}}{|X(\varepsilon_{F})|} \{ \pi \rho_{d}(\varepsilon_{F}) \cos \eta(\varepsilon_{F}) - F_{d}^{R}(\varepsilon_{F}) \sin \eta(\varepsilon_{F}) \}$$
(C.1)

where we have used definitions (B.4).

Now neglecting mixing terms in expression (B.9) (which give higher order contributions) one obtains:

$$\cos \eta(\omega) = \frac{-V_{dd} F_{d}^{R}(\omega)}{|1 - V_{dd} F_{d}(\omega)|}$$

$$\sin \eta(\omega) = -\frac{V_{dd} \pi \rho_{d}(\omega)}{|1 - V_{dd} F_{d}(\omega)|}$$
(C.2)

Substituing (C.2) into (C.1) and neglecting  $|V_{sd}|^2$  contributions in  $|X(\epsilon_F)|$  one gets:

$$\Delta r_0 = Ac \frac{|V_{sd}|^2}{|1 - V_{dd} F_d(\epsilon_F)|^2} \{ \pi \rho_d(\epsilon_F) (1 - V_{dd} F_d^R(\epsilon_F)) + \pi \rho_d(\epsilon_F) V_{dd} F_d^R(\epsilon_F) \}$$

= Ac 
$$\frac{|V_{sd}|^2 \pi \rho_d(\epsilon_F)}{|1 - V_{dd} F_d(\epsilon_F)|^2}$$

Finally:

$$\Delta r_{o} = Ac \frac{\pi |V_{sd}|^{2} \rho_{d}(\epsilon_{F})}{\left[1 - V_{dd} F_{d}^{R}(\epsilon_{F})\right]^{2} + \left[\pi V_{dd} \rho_{d}(\epsilon_{F})\right]^{2}}$$
 (C.3)

which is the result obtained in ref. 5.

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