NOTAS DE FÍSICA

VOLUME XXI NÚMERO 12

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Notas de Física - Volume XXI - Nº 12

REMARKS ON THE EFFECT OF POTENTIAL SCATTERING ON THE SPIN POLARIZATION*

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(Received 6th December 1973)

ABSTRACT

The conduction electron spin polarization, produced by a magnetic rare-earth impurity in a transition metal-like host, is calculated, using the Green's function formalism. The s and d magnetization are obtained to first order in the exchange parameters. Corrected susceptibilities are derived, which includes the difference in valence between impurity and host ions, via the phase-shifts associated to the spin independent potential.

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** To be submitted for publication to Physica Status Solidi.

I. INTRODUCTION

The conduction electron spin polarization associated to a localized spin embedded in a metallic environment has been the subject of much work[1,2]. In particular the combined effect of a charge impurity and a localized spin is a quite interesting problem.

When a magnetic rare-earth impurity is placed in a rare-earth metallic host (e.g. Gd in Lu) there occurs no significant change on the spin independent potential, so the scattering processes involving conduction states take place only via an exchange coupling among the localized spin and the sea of the conduction electrons. However, the situation becomes different if we consider an f-moment impurity placed in a normal or transitional metal. An important effect arises from the fact that the impurity introduces also a charge difference. One expects then additional scattering due to the impurity potential, the conduction states being now scattered simultaneously by the exchange coupling and a spin independent potential.

Blandin and Campbell [3] have recently discussed the effect of a localized potential acting on a s-like band which is polarized by the spin impurity. Our purpose is to discuss the electron spin polarization induced by a rare-earth magnetic impurity in a transition metal-like system.

The plan of this paper is a follows: in Sec. II we formulate the problem under the assumptions that screening is entirely performed by the d-electrons and the mixing between s and d-bands induced by the impurity occurs only at the impurity site. We calculate the Green's s and d-electron propagators and, in order to compute the spin dependent impurity effects, one developes a first order (on J parameters) perturbative approach. In Sec. III we calculate the s and d magnetizations in terms of the phase-shifts [4] associated to spin independent scattering. Some limiting cases are presented.

II) FORMULATION OF THE PROBLEM

a) Hamiltonian of the system

Consider a system of conduction s and d electrons described by two overlapping bands (which for simplicity we assume non-hybridized) and an impurity, placed at the origin, which exhibits a localized magnetic moment (say, an f-moment).

We start describing the host s and d conduction states; in the Wannier representation the unperturbed Hamiltonian reads:

$$\mathcal{H}_0 = \sum_{ij\sigma} T_{ij}^{(s)} c_{i\sigma}^+ c_{j\sigma} + \sum_{ij\sigma} T_{ij}^{(d)} d_{i\sigma}^+ d_{j\sigma} \tag{1}$$

The perturbative charge potential introduced by the impurity gives the terms

$$\mathcal{H}_{pot}^{imp} = \sum_{\sigma} \{V_{dd}\, d_{o\sigma}^+ d_{o\sigma} + V_{sd}\, c_{o\sigma}^+ d_{o\sigma} + V_{ds}\, d_{o\sigma}^+ c_{o\sigma}\} \tag{2}$$

The above terms involves two effects: firstly the excess charge due to the impurity introduces an extra potential which is assumed to act only on the d-electrons at the origin. Screening is then performed almost entirely by the d-states [5] . Furthermore, the s-d hybridization between s and d bands is induced by this impurity potential and occurs only at the impurity site [5].

Finally, the impurity spin is coupled to the conduction states through:

$$\mathcal{H}^{imp}_{exch} = \sum_{ij\sigma} J^{(s)}(R_i,R_j)\sigma <S^z> c^+_{i\sigma} c_{j\sigma} + \sum_{ij\sigma} J^{(d)}(R_i,R_j)\, \sigma <S^z> d^+_{i\sigma} d_{j\sigma} \qquad (3)$$

where $J^{(\lambda)}(R_i,R_j)$, $\lambda = s,d$ is defined by:

$J^{(\lambda)}(R_i,R_j) = \sum_{k,k'} J^{(\lambda)}(k, k') e^{-ik.R_i} e^{ik'.R_j}$ (a k, k' dependent exchange coupling being assumed).

Thus, the complete Hamiltonian is written as:

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

In order to calculate the spin polarization associated to $<S^z>$ one needs the propagators $G^{ss}_{ij}(\omega) = <<c_{i\sigma};c^+_{j\sigma}>>_\omega$ and $G^{dd}_{ij}(\omega) = <<d_{i\sigma};d^+_{j\sigma}>>_\omega$ These propagators are calculated to first order in the exchange parameters.

b) Determination of the equations of motion

Using the Hamiltonian (4) one gets:

$$\omega G^{dd}_{ij}(\omega) = \frac{1}{2\pi}\delta_{ij} + \sum_\ell T^{(d)}_{i\ell} G^{dd}_{\ell j}(\omega) + V_{dd}\,\delta_{io} G^{dd}_{ij}(\omega) + V_{ds}\,\delta_{io} G^{sd}_{ij}(\omega) +$$

$$+ \sum_\ell J^{(d)}(R_i,R_j) <S^z>\sigma\, G^{dd}_{\ell j}(\omega) \qquad (5.a)$$

$$(5.b)$$

$$\omega G^{sd}_{ij}(\omega) = \sum_\ell T^{(s)}_{i\ell} G^{sd}_{\ell j}(\omega) + V_{sd}\,\delta_{io} G^{dd}_{ij}(\omega) + \sum_\ell J^{(s)}(R_i,R_\ell) <S^z>\sigma\, G^{sd}_{\ell j}(\omega)$$

The coupled equations (5.a) and (5.b) determine completely the propagator $G_{ij}^{dd}(\omega)$.

Similarly:

$$\omega\, G_{ij}^{ss}(\omega) = \frac{1}{2\pi}\delta_{ij} + \sum_{\ell} T_{i\ell}^{(s)} G_{\ell j}^{ss}(\omega) + V_{sd}\,\delta_{io}\, G_{ij}^{ds}(\omega) + \sum_{\ell} J^{(s)}(R_i,R_\ell)\langle S^z\rangle\sigma G_{\ell j}^{ss}(\omega) \tag{6.a}$$

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

$$+ \sum_{\ell} J^{(d)}(R_i,R_\ell)\ \langle S^z\rangle\sigma\ G_{\ell j}^{ds}(\omega) \tag{6.b}$$

determine the propagator $G_{ij}^{ss}(\omega)$.

c) <u>Calculation of the d-electron propagator in the Bloch representation.</u>

Fourier transforming equations (5.a) and (5.b) one has:

$$(\omega-\varepsilon_k^{(d)})\ G_{kk'}^{dd}(\omega) = \frac{1}{2\pi}\ \delta_{kk'} + V_{dd}\sum_{k''} G_{k''k'}^{dd}(\omega) + V_{ds}\sum_{k''} G_{k''k'}^{sd}(\omega) + $$

$$+ \sum_{k''} J^{(d)}(k,k'')\ \langle S^z\rangle\sigma\ G_{k''k'}^{dd}(\omega) \tag{7.a}$$

$$(\omega-\varepsilon_k^{(s)})G_{kk'}^{sd}(\omega) = V_{sd}\sum_{k''} G_{k''k'}^{dd}(\omega) + \sum_{k''} J^{(s)}(k,k'')\ \langle S^z\rangle\sigma\ G_{k''k'}^{sd}(\omega) \tag{7.b}$$

Introducing the notation:

$$g_{k'}^{dd}(\omega) = \sum_{k''} G_{k''k'}^{dd}(\omega) \tag{8}$$

$$g^{sd}_{k'}(\omega) = \sum_{k''} G^{sd}_{k''k'}(\omega)$$

$$\overset{(d)dd}{x}_{kk'}(\omega) = \sum_{k''} J^{(d)}(k,k'') \langle S^z \rangle \sigma \, G^{dd}_{k''k'}(\omega)$$

$$\overset{(s)sd}{x}_{kk'}(\omega) = \sum_{k''} J^{(s)}(k,k'') \langle S^z \rangle \sigma \, G^{sd}_{k''k'}(\omega) \tag{8}$$

equations (7.a) and (7.b) become:

$$G^{dd}_{kk'}(\omega) = \frac{1}{2\pi} \delta_{kk'} \frac{1}{\omega-\varepsilon^{(d)}_k} + \frac{V_{dd}}{\omega-\varepsilon^{(d)}_k} g^{dd}_{k'}(\omega) + \frac{V_{ds}}{\omega-\varepsilon^{(d)}_k} g^{sd}_{k'}(\omega) +$$

$$+ \frac{1}{\omega-\varepsilon^{(d)}_k} \overset{(d)dd}{x}_{kk'}(\omega) \tag{9.a}$$

$$G^{sd}_{kk'}(\omega) = \frac{V_{sd}}{\omega-\varepsilon^{(s)}_k} g^{dd}_{k'}(\omega) + \frac{1}{\omega-\varepsilon^{(s)}_k} \overset{(s)sd}{x}_{kk'}(\omega) \tag{9.b}$$

(c.i) <u>Zero order solution</u>

Taking $J^{(s)} = J^{(d)} = 0$, one has: (10.a)

$$G^{dd(o)}_{kk'}(\omega) = \frac{1}{2\pi} \delta_{kk'} \frac{1}{\omega-\varepsilon^{(d)}_k} + \frac{V_{dd}}{\omega-\varepsilon^{(d)}_k} g^{dd(o)}_{k'}(\omega) + \frac{V_{ds}}{\omega-\varepsilon^{(d)}_k} g^{sd(o)}_{k'}(\omega)$$

and:

$$G^{sd(o)}_{kk'}(\omega) = \frac{V_{sd}}{\omega-\varepsilon^{(s)}_k} g^{dd(o)}_{k'}(\omega) \tag{10.b}$$

Introducing the definition:

$$F_{\lambda}(\omega) = \sum_{k} \frac{1}{\omega - \varepsilon_k^{(\lambda)}} , \qquad \lambda = \text{ s or d} \tag{11}$$

it follows from (10.a) and (10.b):

$$g_{k'}^{dd(o)}(\omega) = \frac{1}{2\pi} \frac{1}{1 - V_{dd} F_d(\omega) - |V_{sd}|^2 F_s(\omega) F_d(\omega)} \frac{1}{\omega - \varepsilon_{k'}^{(d)}} \tag{12.a}$$

$$g_{k'}^{sd(o)}(\omega) = \frac{1}{2\pi} \frac{V_{sd} F_s(\omega)}{1 - V_{dd} F_d(\omega) - |V_{sd}|^2 F_s(\omega) F_d(\omega)} \frac{1}{\omega - \varepsilon_{k'}^{(d)}} \tag{12.b}$$

Hence, the zero order propagator $G_{kk'}^{dd(o)}(\omega)$ is:

$$G_{kk'}^{dd(o)}(\omega) = \frac{1}{2\pi} \frac{\delta_{kk'}}{\omega - \varepsilon_k^{(d)}} + \frac{1}{2\pi} \frac{1}{\omega - \varepsilon_k^{(d)}} T^{dd}(\omega) \frac{1}{\omega - \varepsilon_{k'}^{(d)}} \tag{13.a}$$

and for the zero order propagator $G_{kk'}^{dd(o)}(\omega)$, one has :

$$G_{kk'}^{sd(o)}(\omega) = \frac{1}{2\pi} \frac{1}{\omega - \varepsilon_k^{(s)}} T^{sd}(\omega) \frac{1}{\omega - \varepsilon_{k'}^{(d)}} \tag{13.b}$$

where we have defined:

$$T^{dd}(\omega) = \frac{V_{dd} + |V_{sd}|^2 F_s(\omega) F_d(\omega)}{1 - V_{dd} F_d(\omega) - |V_{sd}|^2 F_d(\omega) F_s(\omega)} \tag{14-a}$$

$$T^{\lambda\mu}(\omega) = \frac{V_{\lambda\mu}}{1 - V_{dd}\, F_d(\omega) - |V_{sd}|^2\, F_d(\omega)\, F_s(\omega)} \quad ; (\lambda,\mu = s,d,\ \lambda \neq \mu)$$

(14.b)

It should be emphasized that equation (13.a) provides the exact solution for spin independent impurity effects, the strength of the V_{dd} scattering being determined through the screening condition of the extra charge introduced by the impurity [6].

(c.ii) First order perturbation solution

We solve in this paragraph, to first order in the exchange parameters $J^{(\lambda)}$, $(\lambda = s,d)$, the propagator $G^{dd}_{kk'}(\omega)$; from equations (7) one gets the following results:

$$G^{dd(1)}_{kk'}(\omega) = \frac{V_{dd}}{\omega-\varepsilon^{(d)}_k}\, g^{dd(1)}_{k'}(\omega) + \frac{V_{ds}}{\omega-\varepsilon^{(d)}_k}\, g^{sd(1)}_{k'}(\omega) + \frac{1}{\omega-\varepsilon^{(d)}_k}\, x^{(d)dd(1)}_{kk'}(\omega)$$

(15.a)

$$G^{sd(1)}_{kk'}(\omega) = \frac{V_{sd}}{\omega-\varepsilon^{(s)}_k}\, g^{dd(1)}_{k'}(\omega) + \frac{1}{\omega-\varepsilon^{(s)}_k}\, x^{(s)sd(1)}_{kk'}(\omega) \qquad (15.b)$$

Let us introduce the notation:

$$\gamma^{d(1)}_{k'}(\omega) = \sum_k \frac{1}{\omega-\varepsilon^{(d)}_k}\, x^{(d)dd(1)}_{kk'}(\omega) \qquad (16)$$

$$\gamma_{k'}^{s(1)}(\omega) = \sum_k \frac{1}{\omega - \varepsilon_k^{(s)}} x_{kk'}^{(s)sd(1)}(\omega) \tag{16}$$

where in the $x_{kk'}^{'s}$ the corresponding propagators should be taken to zero order, and consequently these quantities are known.

From equations (15) one has:

$$g_{k'}^{dd(1)}(\omega) = \frac{\gamma_{k'}^{d(1)}(\omega) + V_{ds} F_s(\omega) \gamma_{k'}^{s(1)}(\omega)}{1 - V_{dd} F_d(\omega) - |V_{sd}|^2 F_s(\omega) F_d(\omega)} \tag{17.a}$$

$$g_{k'}^{sd(1)}(\omega) = \frac{(1 - V_{dd} F_d(\omega)) \gamma_{k'}^{s(1)}(\omega) + V_{sd} F_s(\omega) \gamma_{k'}^{d(1)}(\omega)}{1 - V_{dd} F_d(\omega) - |V_{sd}|^2 F_s(\omega) F_d(\omega)} \tag{17.b}$$

$$G_{kk'}^{dd(1)}(\omega) = \frac{1}{\omega - \varepsilon_k^{(d)}} x_{kk'}^{(d)dd(1)}(\omega) + \frac{1}{\omega - \varepsilon_k^{(d)}} T^{dd}(\omega) \gamma_{k'}^{d(1)}(\omega) +$$

$$+ \frac{1}{\omega - \varepsilon_k^{(d)}} \frac{V_{ds} \gamma_{k'}^{s(1)}(\omega)}{1 - V_{dd} F_d(\omega) - |V_{sd}|^2 F_s(\omega) F_d(\omega)} \tag{18}$$

Performing explicit calculations involving $x_{kk'}^{(d)dd(1)}(\omega)$ $\gamma_{k'}^{d(1)}(\omega)$, $\gamma_{k'}^{s(1)}(\omega)$

and after some algebraic manipulations, one finds the final result for the first order correction:

$$G^{dd(1)}_{k+q,k}(\omega) = \frac{1}{2\pi} \frac{1}{\omega - \varepsilon^{(d)}_{k+q}} J^{(d)}(k+q,k) \langle S^z\rangle\sigma \frac{1}{\omega - \varepsilon^{(d)}_{k}} +$$

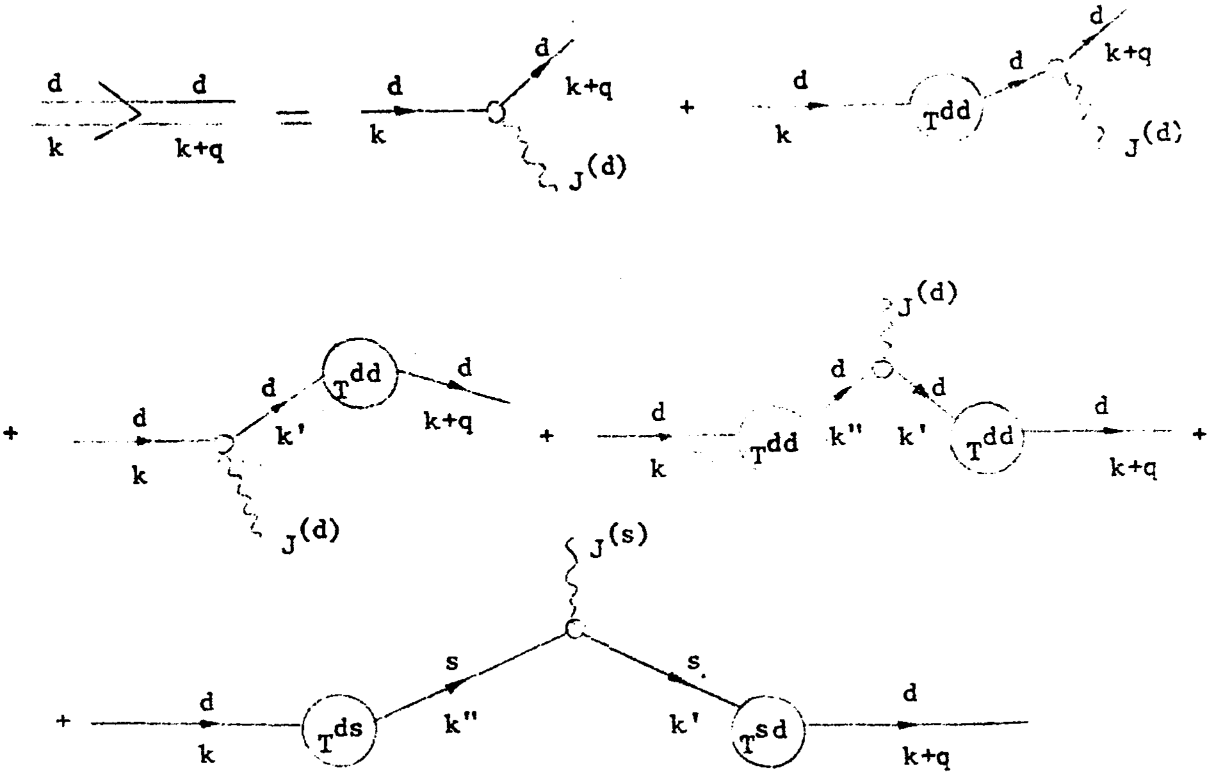
$$+ \frac{1}{2\pi} \frac{1}{\omega-\varepsilon^{(d)}_{k+q}} \sum_{k'} J^{(d)}(k+q,k') \langle S^z\rangle\sigma \frac{1}{\omega-\varepsilon^{(d)}_{k'}} T^{dd}(\omega) \frac{1}{\omega-\varepsilon^{(d)}_{k}} +$$

$$+ \frac{1}{2\pi} \frac{1}{\omega - \varepsilon^{(d)}_{k+q}} T^{dd}(\omega) \sum_{k'} \frac{1}{\omega - \varepsilon^{(d)}_{k'}} J^{(d)}(k',k) \langle S^z\rangle\sigma \frac{1}{\omega - \varepsilon^{(d)}_{k}} +$$

$$+ \frac{1}{2\pi} \frac{1}{\omega-\varepsilon^{(d)}_{k+q}} T^{dd}(\omega) \sum_{k'k''} \frac{1}{\omega-\varepsilon^{(d)}_{k'}} J^{(d)}(k',k'') \langle S^z\rangle\sigma \frac{1}{\omega-\varepsilon^{(d)}_{k''}} T^{dd}(\omega) \frac{1}{\omega-\varepsilon^{(d)}_{k}} +$$

$$+ \frac{1}{2\pi} \frac{1}{\omega-\varepsilon^{(d)}_{k+q}} T^{ds}(\omega) \sum_{k'k''} \frac{1}{\omega-\varepsilon^{(s)}_{k'}} J^{(s)}(k',k'') \langle S^z\rangle\sigma \frac{1}{\omega-\varepsilon^{(s)}_{k''}} T^{sd}(\omega) \frac{1}{\omega-\varepsilon^{(d)}_{k}} \tag{19}$$

In a diagram picture equation (19) looks as:



where we adopt the following notation:

〰 stands for the exchange coupling $J^{(s)}$ or $J^{(d)}$, T^{dd} T^{sd} and T^{ds} are the collision matrices (T-matrices), corresponding respectively to intra d-scattering and s-d scattering.

A convenient approximation is to regard the exchange interaction as being k,k' independent so that: $J^{(\lambda)}(k,k')=J^{(\lambda)}$, $(\lambda=s,d)$. In this simplified situation, the propagator $G^{dd(\lambda)}_{k+q,k}(\omega)$ reads:

$$G^{dd}_{k+q,k}(\omega) = \frac{1}{2\pi} \langle S^z \rangle \sigma \frac{1}{\omega-\varepsilon^{(d)}_{k+}} \frac{J^{(d)} + J^{(s)}|V_{sd}|^2 \ |F_s(\omega)|^2}{\left[1-V_{dd}\ F_d(\omega)-|V_{ds}|^2 F_s(\omega)\ F_d(\omega)\right]^2} \frac{1}{\omega-\varepsilon^{(d)}_{k}} \qquad (20)$$

(d) Calculation of the s-electron propagator in the Bloch representation

The approach is absolutely similar to the paragraph (c). Fourier transforming equations (6.a), (6.b), one has:

$$G^{ss}_{kk'}(\omega) = \frac{1}{2\pi}\,\frac{1}{\omega - \varepsilon_k^{(s)}} + \frac{1}{\omega - \varepsilon_k^{(s)}}\, g^{ds}_{k'}(\omega) + \frac{1}{\omega - \varepsilon_k^{(s)}}\, \chi^{(s)ss}_{kk'}(\omega) \qquad (21.a)$$

$$G^{ds}_{kk'}(\omega) = \frac{1}{\omega - \varepsilon_k^{(d)}}\, g^{ds}_{k'}(\omega) + \frac{1}{\omega - \varepsilon_k^{(d)}}\, g^{ss}_{k'}(\omega) + \frac{1}{\omega - \varepsilon_k^{(d)}}\, \chi^{(d)ds}_{kk'}(\omega) \qquad (21.b)$$

where:

$$g^{ss}_{k'}(\omega) = \sum_{k''} G^{ss}_{k''k''}(\omega)$$

$$g^{ds}_{k'}(\omega) \quad \sum_{k''} G^{ds}_{k''k'}(\omega)$$

$$\chi^{(s)ss}_{kk'}(\omega) = \sum_{k''} J^{(s)}(k,k'')\, \langle S^z\rangle\sigma \;\; G^{ss}_{k''k'}(\omega) \qquad (22)$$

$$\chi^{(d)ds}_{kk'}(\omega) = \sum_{k''} J^{(d)}(k,k'')\, \langle S^z\rangle\sigma \; G^{ds}_{k''k'}(\omega)$$

(d.i) Zero order solution for the coupled system (21)

Taking again $J^{(s)} = J^{(d)} = 0$, one obtains:

$$G^{ss(o)}_{kk'}(\omega) = \frac{1}{2\pi}\;\frac{\delta_{kk'}}{\omega-\varepsilon^{(s)}_k} + \frac{V_{ds}}{\omega-\varepsilon^{(s)}_k}\; g^{ds(o)}_{k'}(\omega) \tag{23.a}$$

$$G^{ds(o)}_{kk'}(\omega) = \frac{V_{dd}}{\omega-\varepsilon^{(d)}_k}\; g^{ds(o)}_{k'}(\omega) \tag{23.b}$$

which leads to:

$$g^{ss(o)}_{k'}(\omega) = \frac{1}{2\pi}\;\frac{1 - V_{dd}\,F_d(\omega)}{1 - V_{dd}\,F_d(\omega) - |V_{sd}|^2\,F_s(\omega)\,F_d(\omega)}\;\frac{1}{\omega-\varepsilon^{(s)}_{k'}} \tag{24.a}$$

$$g^{ds(o)}_{k'}(\omega) = \frac{1}{2\pi}\;\frac{V_{ds}\,F_d(\omega)}{1 - V_{dd}\,F_d(\omega) - \;V_{sd}\;\,F_s(\omega)\,F_d(\omega)}\;\frac{1}{\omega-\varepsilon^{(s)}_{k'}} \tag{24.b}$$

Hence, the zero order propagator $G^{ss(o)}_{kk'}(\omega)$ reads:

$$G^{ss(o)}_{kk'}(\omega) = \frac{1}{2\pi}\;\frac{\delta_{kk'}}{\omega-\varepsilon^{(s)}_k} + \frac{1}{2\pi}\;\frac{1}{\omega-\varepsilon^{(s)}_k}\;T^{ss}(\omega)\;\frac{1}{\omega-\varepsilon^{(s)}_{k'}} \tag{25}$$

where:

$$T^{ss}(\omega) = \frac{|V_{sd}|^2\,F_d(\omega)}{1 - V_{dd}F_d(\omega) - |V_{sd}|^2\,F_s(\omega)F_d(\omega)} \tag{26}$$

(d.ii) First order perturbation solution

Solving equations (21) to first order in the exchange parameters $J^{(\lambda)}$, (λ = s, d) one has:

$$G_{kk'}^{ss(1)}(\omega) = \frac{V_{sd}}{\omega-\varepsilon_k^{(s)}}\, g_{k'}^{(1)ds}(\omega) + \frac{1}{\omega-\varepsilon_k^{(s)}}\, x_{kk'}^{(s)ss(1)}(\omega) \quad (27.a)$$

$$G_{kk'}^{ds(1)}(\omega) = \frac{V_{dd}}{\omega-\varepsilon_k^{(d)}}\, g_{k'}^{ds(1)}(\omega) + \frac{V_{ds}}{\omega-\varepsilon_{k'}^{(d)}}\, g_{k'}^{ss(1)}(\omega) + \frac{1}{\omega-\varepsilon_k^{(d)}}\, x_{kk'}^{(d)ds(1)}(\omega) \quad (27.b)$$

Introducing the notation:

$$\beta_{k'}^{s(1)}(\omega) = \sum_k \frac{1}{\omega-\varepsilon_k^{(s)}}\, x_{kk'}^{(s)ss(1)}(\omega) \quad (28.a)$$

$$\beta_{k'}^{d(1)}(\omega) = \sum_k \frac{1}{\omega-\varepsilon_k^{(d)}}\, x_{kk'}^{(d)ds(1)}(\omega) \quad (28.b)$$

and using equations (27), one gets:

$$g_{k'}^{ds(1)}(\omega) = \frac{\beta_{k'}^{d(1)}(\omega) + V_{ds}F_d(\omega)\,\beta_{k'}^{s(1)}(\omega)}{1 - V_{dd}F_d(\omega) - |V_{sd}|^2\, F_s(\omega)\, F_d(\omega)} \quad (29)$$

Thus, the $G_{kk'}^{ss(1)}(\omega)$ propagator is written as:

$$G^{ss(1)}_{kk'}(\omega) = \frac{1}{\omega-\varepsilon^{(s)}_k} \; x^{(s)ss(1)}_{kk'}(\omega) + \frac{1}{\omega - \varepsilon^{(s)}_k} T^{sd}(\omega)\; \beta^{d(1)}_{k'}(\omega) + \tag{30}$$

$$+ \frac{1}{\omega - \varepsilon^{(s)}_k} T^{sd}(\omega)\; V_{ds}\; F_d(\omega)\; \beta^{s(1)}_{k'}(\omega)$$

Again we must proceed some algebraic manipulations involving expressions like $x^{ss(1)}_{kk'}(\omega)$, $\beta^{s(1)}_{k'}(\omega)$, $\beta^{d(1)}_{k'}(\omega)$, and one has the final result for the first order corrections, namely:

$$G^{ss(1)}_{k+q,k}(\omega) = \frac{1}{2\pi} \frac{1}{\omega-\varepsilon^{(s)}_{k+q}} J^{(s)}(k+q,k) \; \langle S^z\rangle\sigma \; \frac{1}{\omega-\varepsilon^{(s)}_k} + \tag{31}$$

$$+ \frac{1}{2\pi}\frac{1}{\omega-\varepsilon^{(s)}_{k+q}} \sum_{k'} J^{(s)}(k+q,k') \; \langle S^z\rangle\sigma \; \frac{1}{\omega-\varepsilon^{(s)}_{k'}} T^{ss}(\omega) \; \frac{1}{\omega-\varepsilon^{(s)}_k} +$$

$$+ \frac{1}{2\pi} \frac{1}{\omega-\varepsilon^{(s)}_{k+q}} T^{ss}(\omega) \sum_{k'} \frac{1}{\omega-\varepsilon^{(s)}_{k'}} J^{(s)}(k',k) \; \langle S^z\rangle\sigma \; \frac{1}{\omega-\varepsilon^{(s)}_k} +$$

$$+ \frac{1}{2\pi} \frac{1}{\omega-\varepsilon^{(s)}_{k+q}} T^{ss}(\omega) \sum_{k',k''} \frac{1}{\omega-\varepsilon^{(s)}_{k'}} J^{(s)}(k',k'') \; \langle S^z\rangle\sigma \; \frac{1}{\omega-\varepsilon^{(s)}_{k''}} T^{ss}(\omega) \; \frac{1}{\omega-\varepsilon^{(s)}_k} +$$

$$+ \frac{1}{2\pi} \frac{1}{\omega-\varepsilon^{(s)}_{k+q}} T^{sd}(\omega) \sum_{k',k''} \frac{1}{\omega-\varepsilon^{(d)}_{k'}} J^{(d)}(k',k'') \; \langle S^z\rangle\sigma \; \frac{1}{\omega-\varepsilon^{(d)}_{k''}} \; T^{ds}(\omega) \; \frac{1}{\omega-\varepsilon^{(s)}_k}$$

Equation (31) corresponds for s-electrons to equation (19) which holds for d-electrons and the diagrammatic expansion is formally identical. In the case of k-independent coupling parameter $J^{(s)}$, equation (31) simplifies to:

$$G^{ss(1)}_{k+q,k}(\omega) = \frac{1}{2\pi}\,\frac{1}{\omega-\varepsilon^{(s)}_{k+q}}\,\frac{J^{(s)}\,\langle S^z\rangle\sigma\,[1-V_{dd}F_d(\omega)]^2}{\left[1 - V_{dd}\,F_d(\omega) - |V_{sd}|^2\,F_s(\omega)\,F_d(\omega)\right]^2}\,\frac{1}{\omega-\varepsilon^{(s)}_k} +$$

$$+\frac{1}{2\pi}\,\frac{1}{\omega-\varepsilon^{(s)}_k}\,\frac{J^{(d)}\,\langle S^z\rangle\sigma\,|V_{sd}|^2\,[F_d(\omega)]^2}{\left[1 - V_{dd}\,F_d(\omega) - |V_{sd}|^2\,F_s(\omega)\,F_d(\omega)\right]^2}\,\frac{1}{\omega-\varepsilon^{(s)}_k} \qquad (32)$$

III) SPIN POLARIZATION

It will be supposed for simplicity, that $J^{(\lambda)}(\lambda = s, d)$ is k-independent; we expect that such approximation will not destroy the main features of the problem. Thus, one adopts equations (20) and (32) to describe the propagations of d and s-electrons respectively.

Let us denote:

$$1 - V_{dd}\,F_d(\omega) = K(\omega)$$

$$1 - V_{dd}\,F_d(\omega) - |V_{sd}|^2\,F_s(\omega)\,F_d(\omega) = X(\omega)$$

Introducing the phase shifts [4], one has:

$$\begin{aligned} F_s(\omega) &= |F_s(\omega)|\,e^{-i\delta_s(\omega)} \\ F_d(\omega) &= |F_d(\omega)|\,e^{-i\delta_d(\omega)} \\ K(\omega) &= |K(\omega)|\,e^{-i\eta_{dd}(\omega)} \\ X(\omega) &= |X(\omega)|\,e^{-i\eta(\omega)} \end{aligned} \qquad (33)$$

where $|F_s(\omega)|$, $|F_d(\omega)|$, $|K(\omega)|$, $|X(\omega)|$, $\delta_s(\omega)$, $\delta_d(\omega)$, $\eta_{dd}(\omega)$, $\eta(\omega)$ are defined in Appendix A.

(a) Calculation of the d magnetization

If one takes into account definitons (33), equation (20) reads:

$$G^{dd(1)}_{k+q,k}(\omega_{\pm}) = \frac{1}{2\pi} <S^z>\sigma \frac{1}{\omega_{\pm}-\varepsilon^{(d)}_{k+q}} |t^{dd}(\omega)| J^{(d)} \frac{1}{\omega_{\pm}-\varepsilon^{(d)}_{k}} e^{2 i\eta(\omega)} +$$

$$+ \frac{1}{2\pi} <S^z>\sigma \frac{1}{\omega_{\pm}-\varepsilon^{(d)}_{k+q}} |t^{ds}(\omega)| J^{(s)} \frac{1}{\omega_{\pm}-\varepsilon^{(d)}_{k}} e^{2i\left[\eta(\omega)-\delta_s(\omega)\right]} ,$$

$$\omega_{\pm} = \omega \pm i\delta \qquad (34)$$

where:

$$|t^{dd}(\omega)| = \frac{1}{|X(\omega)|^2}$$

$$|t^{ds}(\omega)| = |V_{sd}|^2 \frac{|F_s(\omega)|^2}{|X(\omega)|^2}$$

Remembering that:

$$\sum_k F_{\omega} \left[G^{dd(1)}_{k+q,k}(\omega)\right] = \Delta n^{\sigma(d)}_q$$

the symbol F_{ω} being defined as usually by $i \int_{-\infty}^{+\infty} d\omega\, f(\omega) \left[G(\omega+i\delta)-G(\omega-i\delta)\right]$, one obtains after some algebra: ($f(\omega)$ is the Fermi-Dirac distribution function)

$$\Delta n_q^{\sigma}(\omega) = \langle S^z\rangle \sigma J^{(d)} \sum_k \frac{f_1^{dd}(\varepsilon_{k+q}^{(d)}) - f_1^{dd}(\varepsilon_k^{(d)})}{\varepsilon_{k+q}^{(d)} - \varepsilon_k^{(d)}} +$$

$$+ \langle S^z\rangle \sigma J^{(d)} \sum_k \frac{f_2^{dd}(\varepsilon_{k+q}^{(d)}) - f_2^{dd}(\varepsilon_k^{(d)})}{\varepsilon_{k+q}^{(d)} - \varepsilon_k^{(d)}} +$$

$$+ \langle S^z\rangle \sigma\, J^{(s)} \sum_k \frac{f_1^{ds}(\varepsilon_{k+q}^{(d)}) - f_1^{ds}(\varepsilon_k^{(d)})}{\varepsilon_{k+q}^{(d)} - \varepsilon_k^{(d)}} +$$

$$+ \langle S^z\rangle \sigma\, J^{(s)} \sum_k \frac{f_2^{ds}(\varepsilon_{k+q}^{(d)}) - f_2^{ds}(\varepsilon_k^{(d)})}{\varepsilon_{k+q}^{(d)} - \varepsilon_k^{(d)}} \qquad (35)$$

where we construct the functions:

$$f_1^{dd}(\omega) = |t^{dd}(\omega)| \cos [2\eta(\omega)] \; f(\omega)$$

$$f_1^{ds}(\omega) = |t^{ds}(\omega)| \cos [2\eta(\omega) - 2\,\delta_s(\omega)] \; f(\omega)$$

$$f_2^{dd}(\omega) = \frac{1}{\pi} \; P \int \frac{d\omega' \; f(\omega) \; |t^{dd}(\omega)| \sin [2\,\eta(\omega)]}{\omega' - \omega} \qquad (36)$$

$$f_2^{ds}(\omega) = \frac{1}{\pi} \; P \int \frac{d\omega' \; f(\omega) \; |t^{ds}(\omega)| \sin [2\eta(\omega) - 2\,\delta_s(\omega)]}{\omega' - \omega}$$

In order to rewrite equation (35) in a more compact form we can define the susceptibilities:

$$\chi^{dd}(q) = \sum_k \frac{[f_1^{dd}(\varepsilon_{k+q}^{(d)}) + f_2^{dd}(\varepsilon_{k+q}^{(d)})] - [f_1^{dd}(\varepsilon_k^{(d)}) + f_2^{dd}(\varepsilon_k^{(d)})]}{\varepsilon_{k+q}^{(d)} - \varepsilon_k^{(d)}} \qquad (37.a)$$

$$\chi^{ds}(q) = \sum_k \frac{[f_1^{ds}(\varepsilon_{k+q}^{(d)}) + f_2^{ds}(\varepsilon_{k+q}^{(d)})] - [f_1^{ds}(\varepsilon_k^{(d)}) + f_2^{ds}(\varepsilon_k^{(d)})]}{\varepsilon_{k+q}^{(d)} - \varepsilon_k^{(d)}} \qquad (37.b)$$

Thus, one obtains:

$$m_q^{(d)} = 2 <S^z> J^{(d)} \chi^{dd}(q) + 2 <S^z> J^{(s)} \chi^{ds}(q) \qquad (38)$$

(b) <u>Calculation of the s magnetization</u>

Proceeding exatly as in the case of d-electrons, equation (32) may be rewritten as:

$$G_{k+q,k}^{ss(i)}(\omega_\pm) = \frac{1}{2\pi} <S^z>\sigma \frac{1}{\omega_\pm - \varepsilon_{k+q}^{(s)}} |t^{ss}(\omega)| J^{(s)} \frac{1}{\omega_\pm - \varepsilon_k^{(s)}} e^{\pm 2i[\eta(\omega) - \eta_{dd}(\omega)]} +$$

$$+ \frac{1}{2\pi} <S^z>\sigma \frac{1}{\omega_\pm - \varepsilon_{k+q}^{(s)}} |t^{sd}(\omega)| J^{(d)} \frac{1}{\omega_\pm - \varepsilon_k^{(s)}} e^{\pm 2i[\eta(\omega) - \delta_d(\omega)]} + \qquad (39)$$

$$\omega_\pm = \omega \pm i\delta$$

where:

$$|t^{ss}(\omega)| = \frac{|K(\omega)|^2}{|X(\omega)|^2}$$

$$|t^{sd}(\omega)| = \frac{|F_d(\omega)|^2}{|X(\omega)|^2}$$

The fluctuation of the occupation number is:

$$\Delta n_q^{\sigma(s)} = \langle S^z\rangle\sigma\, J^{(s)} \sum_k \frac{f_1^{ss}(\varepsilon_{k+q}^{(s)}) - f_1^{ss}(\varepsilon_k^{(s)})}{\varepsilon_{k+q}^{(s)} - \varepsilon_k^{(s)}}$$

$$+ \langle S^z\rangle\sigma\, J^{(s)} \sum_k \frac{f_2^{ss}(\varepsilon_{k+q}^{(s)}) - f_2^{ss}(\varepsilon_k^{(s)})}{\varepsilon_{k+q}^{(s)} - \varepsilon_k^{(s)}}$$

$$+ \langle S^z\rangle\sigma\, J^{(d)} \sum_k \frac{f_1^{sd}(\varepsilon_{k+q}^{(s)}) - f_1^{sd}(\varepsilon_k^{(s)})}{\varepsilon_{k+q}^{(s)} - \varepsilon_k^{(s)}}$$

$$+ \langle S^z\rangle\sigma\, J^{(d)} \sum_k \frac{f_2^{sd}(\varepsilon_{k+q}^{(s)}) - f_2^{sd}(\varepsilon_k^{(s)})}{\varepsilon_{k+q}^{(s)} - \varepsilon_k^{(s)}} \qquad (40)$$

where:

$$f_1^{ss}(\omega) = |t^{ss}(\omega)| \cos\left[2\eta(\omega) - 2\,\eta_{dd}(\omega)\right] f(\omega)$$

cont.

$$f_1^{sd}(\omega) = |t^{sd}(\omega)| \cos\left[2\eta(\omega) - 2\,\delta_d(\omega)\right] f(\omega)$$

$$f_2^{ss}(\omega) = \frac{1}{\pi}\, P \int \frac{d\omega'\; f(\omega)\; |t^{ss}(\omega)| \sin\left[2\eta(\omega) - 2\eta_{dd}(\omega)\right]}{\omega' - \omega} \tag{41}$$

$$f_2^{sd}(\omega) = \frac{1}{\pi}\, P \int \frac{d\omega'\; f(\omega)\; |t^{sd}(\omega)| \sin\left[2\eta(\omega) - 2\,\delta_d(\omega)\right]}{\omega' - \omega}$$

Defining the susceptibilities:

$$\chi^{ss}(q) = \sum_k \frac{\left[f_1^{ss}(\varepsilon_{k+q}^{(s)}) + f_2^{ss}(\varepsilon_{k+q}^{(s)})\right] - \left[f_1^{ss}(\varepsilon_k^{(s)}) + f_2^{ss}(\varepsilon_k^{(s)})\right]}{\varepsilon_{k+q}^{(s)} - \varepsilon_k^{(s)}} \tag{42.a}$$

$$\chi^{sd}(q) = \sum_k \frac{\left[f_1^{sd}(\varepsilon_{k+q}^{(s)}) + f_2^{sd}(\varepsilon_{k+q}^{(s)})\right] - \left[f_1^{sd}(\varepsilon_k^{(s)}) + f_2^{sd}(\varepsilon_k^{(s)})\right]}{\varepsilon_{k+q}^{(s)} - \varepsilon_k^{(s)}} \tag{42.b}$$

one finds the final result for the s magnetization:

$$m_q^{(s)} = 2 \langle S^z \rangle\; J^{(s)}\; \chi^{ss}(q) + 2\langle S^z \rangle\; J^{(d)}\; \chi^{sd}(q) \tag{43}$$

(c) Limiting cases

(c.i) Absence of induced s-d hybridization

In this paragraph we consider the situation where induced s-d mixing vanishes. Although such an assumption seems to be merely academic, (since both V_{sd} and V_{dd} originate in the same potential), this procedure exhibits the behaviour of the s band when isolated from the rest. One has:

$$|t^{ds}(\omega)| = |t^{sd}(\omega)| = 0 \Rightarrow f_1^{ds}(\omega) = f_1^{sd}(\omega) = f_2^{sd}(\omega) = f_2^{ds}(\omega) = 0$$

$$|1 - V_{dd} F_d(\omega)| = |X(\omega)| \Rightarrow |t^{ss}(\omega)| = 1$$

$$\eta_{dd}(\omega) = \eta(\omega) \Rightarrow f_1^{ss}(\omega) = f(\omega)$$

and the susceptibilities (37.b), (42.a), (42.b) reduce to:

$$\chi^{ds}(q) = \chi^{sd}(q) = 0$$

$$\chi^{ss}(q) = \sum_k \frac{f(\varepsilon_{k+q}^{(s)}) - f(\varepsilon_k^{(s)})}{\varepsilon_{k+q}^{(s)} - \varepsilon_k^{(s)}}$$

Thus, the s magnetization becomes:

$$m_q^{(s)} = 2 \langle S^z \rangle J^{(s)} \sum_k \frac{f(\varepsilon_{k+q}^{(s)}) - f(\varepsilon_k^{(s)})}{\varepsilon_{k+q}^{(s)} - \varepsilon_k^{(s)}} \tag{44}$$

which is just the classical independent electron spin polarization due to an external magnetic field. In fact, if we switch-off the induced s-d mixing, the s-like electrons cannot "see" the perturbative charge effects produced by the impurity.

(c.ii) Absence of perturbative charge potential ($V_{dd} = V_{sd} = 0$)

A further simplification occurs when we consider also $V_{dd}=0$. Hence:

$$\eta_{dd}(\omega) = \eta(\omega) = 0$$

$$|t^{dd}(\omega)| = 1$$

which implies that:

$$f_1^{dd}(\omega) = f(\omega)$$

So, one gets for the susceptibility (37.a):

$$\chi^{dd}(q) = \sum_k \frac{f(\varepsilon_{k+q}^{(d)}) - f(\varepsilon_k^{(d)})}{\varepsilon_{k+q}^{(d)} - \varepsilon_k^{(d)}}$$

The d magnetization becomes:

$$m_q^{(d)} = 2 \langle S^z \rangle \sum_k \frac{f(\varepsilon_{k+q}^{(d)}) - f(\varepsilon_k^{(d)})}{\varepsilon_{k+q}^{(d)} - \varepsilon_k^{(d)}} \tag{45}$$

and for the s magnetization one obtains (44). Expressions (44) and (45) are just the usual ones employed in the case of independent bands.

DISCUSSION AND CONCLUSIONS

The effect of a spin independent localized potential acting simultaneously with a localized spin on a band of s-d conduction states, was discussed in terms of the band parameters, impurity matrix elements and the exchange couplings. The general case of k,k' dependent exchange couplings, although more realistic [1], turns out to be mathematically very difficult to handle.

A simplifying approximation of constant $J^{(s)}$ and $J^{(d)}$ was then adopted in order to derive simpler expressions. The main advantage of this simplification is that the usual results for spin polarization problems, namely, the product of an exchange constant times a "susceptibility" charateristic of the host metal, is recovered. Since now the host is perturbed by an extra spin independent potential, the usual form of non-interacting electron susceptibility is not obtained.

However, expressions (42), (37) show that the same formal result is obtained as in the pure host case, provided that "new" Fermi distributions functions are introduced. These new distribution functions include scattering effects through phase-shifts and the strengths of the T-matrices. One consequently associates, in a pictorial fashion, these new functions to "deformations" of the Fermi distribution function due to the scattering via the impurity charge potential. These functions reduce to the Fermi one in the limit of zero charge potential.

A final word is necessary respect to the role of Coulomb interactions. Since the effect of these correlations (besides Hartree-Fock renormalization of energies) is to introduce a new source of scattering through the coupling to occupation number fluctuation [2], the effective impurity potential is now k,k' dependent and only approximate solutions can be obtained (e.g., Born approximation). Hence, the treatment discussed above, excludes strongly exchange enhanced hosts like Pd, for instance. Only formal results (envolving a summation over an infinit series) can be obtained for this general problem, subject to certain assumptions concerning the nature of the screening. [7]

APPENDIX A

PHASE-SHIFT PARAMETERS

Taking into account definition (11), for $\omega \pm i\delta$ in the limit $\delta \to 0$, one has real and imaginary parts. Hence:

$$F_\lambda(\omega \pm i\delta) = F_\lambda^R(\omega) \mp i\, F_\lambda^I(\omega), \quad (\lambda = s,\, d) \tag{A-1}$$

where:

$$F_\lambda^R(\omega) = P \sum_k \frac{1}{\omega - \varepsilon_k^{(\lambda)}} \; ; \quad F_\lambda^I(\omega) = \pi\rho_\lambda\,(\omega) \tag{A-2}$$

$\rho_\lambda(\omega)$ denoting the density of states of conduction electrons. If we introduce the phase shift, one may write:

$$F_\lambda(\omega \pm i\delta) = |F_\lambda(\omega)|\; e^{\mp i\delta_\lambda(\omega)} \tag{A-3}$$

where:

$$|F_\lambda(\omega)| = \left[(F^R(\omega))^2 + (F_\lambda^I(\omega))^2\right]^{1/2} \tag{A-4}$$

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

$$\sin\,\delta_\lambda(\omega) = \frac{F_\lambda^1(\omega)}{|F_\lambda(\omega)|}$$

It is clear that:

$$F_s(\omega\pm i\delta)\ F_d(\omega\pm i\delta) = |F_s(\omega)||F_d(\omega)|\ e^{\mp i\left[\delta_s(\omega) + \delta_d(\omega)\right]} \tag{A-5}$$

Similarly:

$$1 - V_{dd}\ F_d(\omega\pm i\delta) = |1 - V_{dd}\ F_d(\omega)|\ e^{\mp i\eta_{dd}(\omega)} \tag{A-6}$$

where:

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

$$\cos\ \eta_{dd}(\omega) = \frac{1 - V_{dd}\ F_d^R(\omega)}{|1 - V_{dd}\ F_d(\omega)|}$$

$$\sin\ \eta_{dd}(\omega) = -\frac{V_{dd}F_d^I(\omega)}{|1 - V_{dd}\ F_d(\omega)|} \tag{A-7}$$

And finally:

$$1 - V_{dd}F_d(\omega\pm i\delta) - |V_{sd}|^2\ F_s(\omega\pm i\delta)\ F_d(\omega\pm i\delta) = |X(\omega)|\ e^{\mp i\delta(\omega)} \tag{A-8}$$

where:

$$|X(\omega)| = \{[1 - V_{dd} F_d^R(\omega) - |V_{sd}|^2 (F_d^R(\omega) F_s^R(\omega) - F_d^I(\omega) F_s^I(\omega))]^2 +$$

$$+ [V_{dd} F_d^I(\omega) - |V_{sd}|^2 (F_d^R(\omega) F_s^I(\omega) + F_d^I(\omega) F_s^R(\omega))]^2\}^{1/2}$$

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

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

ACKNOWLEDGEMENT

One of the authors (A. Troper) would like to thank Comissão Nacional de Energia Nuclear for research fellowship.

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