

Effect of localized perturbations on the spin polarization: Two-band model

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The conduction-electron spin polarization, induced by a magnetic rare-earth impurity embedded in a transition-metal-like host, is calculated, using the Green's-function formalism. The s and d magnetizations are calculated to first order in the exchange parameters, in terms of partial static susceptibilities $\bar{\chi}^{dd}(\vec{q})$, $\bar{\chi}^{ds}(\vec{q})$, $\bar{\chi}^{sd}(\vec{q})$, and $\bar{\chi}^{ss}(\vec{q})$. These susceptibilities are expressed in terms of the host band structure, phase-shifts, and strength of matrix elements associated to the charge impurity potential and local Coulomb correlation parameter at the impurity site. These results are compared to previous ones and possible applications are discussed.

I. INTRODUCTION

The theoretical study of the conduction-electron spin polarization induced by a local moment involves many aspects, e.g., the discussion of the mechanism of exchange coupling between the localized and conduction electrons,¹ the details of the band structure,² the presence of electron-electron correlations in the conduction states,³⁻⁵ and the combined effect of a charge impurity potential and a localized spin.⁶

In general, the atom which carries the local moment is not identical to the host atoms, and one expects a scattering source arising from the charge difference and the period effects introduced by the impurity.

An interesting example of this situation is a rare-earth impurity embedded in a transition-metal host. Besides the scattering associated with the exchange coupling with the incomplete $4f$ shell, the charge difference between the impurity (trivalent) and the host gives an additional scattering potential for the conduction electrons. On the other hand, one knows that the intra-atomic Coulomb correlations play an important role in narrow d bands. In particular the Coulomb repulsion at the impurity rare-earth site is quite different from that corresponding to the transition-metal host, introducing then another source of scattering.

Blandin and Campbell⁶ have recently discussed the effect of a localized charge potential acting on a free-electron-like band which is polarized via local moments surrounding the impurity charge potential.

Our purpose is to formulate the problem of the electron-spin polarization induced by a rare-earth magnetic impurity in a more complex situation, namely, a transition-metal-like host. We are interested in the physical situation where the magnetic impurity introduces itself, both the spin-dependent and charge potential scattering. So, we study in this two-band system, the combined effects of one-electron charge and spin impurity po-

tentials acting at the same lattice site. The difference of the d -electron Coulomb correlations between the host and the impurity, which introduces an extra potential acting at the impurity site, is also included in this formulation, within the Hartree-Fock scheme. The local f moments are assumed to be associated with localized levels lying well below the conduction s - d bands.

The plan of this paper is as follows: In Sec. II we describe the adopted model Hamiltonian and we obtain the one-electron s - s and d - d propagators using a Green's-function technique due to Zubarev,⁷ discussing the electron-electron correlation at the impurity site within the Hartree-Fock approximation. It should be noted that throughout this work we neglect the intra-atomic Coulomb correlations in the d band. In order to calculate the magnetization induced by the localized moment, one develops a first-order perturbative approach on the exchange parameters; i.e., the impurity spin s - f and d - f exchange fields will be treated as weak perturbations. In that sense, our work is a linear-response calculation of the perturbed electron gas to a field locally applied at the impurity site. In Sec. III we solve the self-consistency problem and calculate the s and d magnetizations in the approximation of neglecting the \vec{k} , \vec{k}' dependence of the exchange integrals. The explicit \vec{k} , \vec{k}' dependence introduces extra difficulties in performing the self-consistency program. These magnetizations are obtained in terms of phase shifts associated with the impurity charge scattering and change in Coulomb correlation parameter. A comparison to previously obtained results by Mills and Lederer⁸ is then made, in the case of decoupled s and d bands (vanishing impurity-induced s - d hybridization) and for static properties. In Sec. IV we calculate the spin polarization at the impurity site, thus complementing some previous results of Blandin and Campbell,⁶ where the charge and spin potentials are located at different sites. In Sec. V we suggest two alternative procedures to estimate the impurity matrix

elements. Finally, Sec. VI is devoted to the general discussions and possible applications.

II. FORMULATION OF PROBLEM

A. Description of model

We adopt a simplified picture to describe a transition-metal host with a rare-earth impurity placed in it:

(i) The unperturbed one-electron Hamiltonian which describes the host s and d conduction states is written, in the Wannier representation,

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

where $c_{i\sigma}^\dagger$ ($d_{i\sigma}^\dagger$) creates a s (d) electron of spin σ at lattice site i and $T_{ij}^{(\lambda)}$ ($\lambda = s$ or d) is the hopping matrix element for λ electrons between the i th and j th sites, $T_{ij}^{(\lambda)}$ being related to the band energy $\epsilon_{\mathbf{k}}^{(\lambda)}$ of the host by

$$T_{ij}^{(\lambda)} = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}}^{(\lambda)} e^{-i\mathbf{k} \cdot (\mathbf{R}_i - \mathbf{R}_j)}, \quad \epsilon_{\mathbf{k}}^{(\lambda)} = \sum_{\mathbf{0}} T_{0\mathbf{0}}^{(\lambda)} e^{i\mathbf{k} \cdot \mathbf{R}_0}.$$

In the host-metal description we neglect hybridization effects in order to simplify the calculation: only impurity-induced mixing will be considered.

(ii) The rare-earth impurity, placed at the origin, is assumed to introduce two types of one-electron perturbations: excess charge effects (through a Friedel type of potential) and spin effects (through the exchange interactions between conduction states and the localized impurity spin). We consider firstly charge effects, which give the terms

$$\mathcal{H}_{\text{ch}}^{\text{imp}} = \sum_{\sigma} V_{dd} n_{0\sigma}^{(d)} + \sum_{\sigma} (V_{sd} c_{0\sigma}^\dagger d_{0\sigma} + V_{ds} d_{0\sigma}^\dagger c_{0\sigma}), \quad (2)$$

$$n_{0\sigma}^{(d)} = d_{0\sigma}^\dagger d_{0\sigma}.$$

In the above Hamiltonian we neglect completely intra- s -band scattering V_{ss} . The phenomenological s - d hybridization between s and d bands is induced by this impurity potential and occurs only at the impurity site. This simplified picture has been used to discuss the resistivity of transition-metal-based alloys.^{9,10} A more detailed description of impurity-potential effects in transition metals has been proposed by Riedinger and Gautier.¹¹ However, for simplicity, we adopt here this model Hamiltonian (2), which we expect describes qualitatively the effects we intend to consider.

(ii) The localized spin is coupled to the conduction states through

$$\mathcal{H}_{\text{ex}}^{\text{imp}} = - \sum_{ij\sigma} J^{(s)}(\mathbf{R}_i, \mathbf{R}_j) \sigma \langle S^x \rangle c_{i\sigma}^\dagger c_{j\sigma} - \sum_{ij\sigma} J^{(d)}(\mathbf{R}_i, \mathbf{R}_j) \sigma \langle S^x \rangle d_{i\sigma}^\dagger d_{j\sigma}, \quad (3)$$

where a \vec{k} , \vec{k}' -dependent exchange coupling is assumed:

$$J^{(\lambda)}(\mathbf{R}_i, \mathbf{R}_j) = \sum_{\vec{k}, \vec{k}'} J^{(\lambda)}(\vec{k}, \vec{k}') e^{-i\vec{k} \cdot \mathbf{R}_i} e^{i\vec{k}' \cdot \mathbf{R}_j}, \quad \lambda = s \text{ or } d;$$

the couplings $J^{(\lambda)}(\vec{k}, \vec{k}')$ correspond to the exchange interaction between the localized f electrons and conduction states, as previously calculated in the literature.¹ As mentioned in the Introduction, in (3) we restrict ourselves to the ionic case and exclude resonant f states as would be expected for Ce impurities.¹² If this is to be included, we do it through the Wolff-Schrieffer transformation.

(iv) It is well known that rare-earth d states ($5d$) are quite different from $3d$ states of usual transition metals or intermetallics. One expects, beside period effects¹³ approximately included in V_{dd} , an important variation of the Coulomb interaction at the impurity site. In the host metal we neglect Coulomb correlations and take them into account only at the impurity site. The Hamiltonian is

$$\mathcal{H}_{\text{Coul}}^{\text{imp}} = \Delta U n_{0i}^{(d)} n_{0i}^{(d)}, \quad \Delta U = U_{\text{imp}} - U_{\text{host}}, \quad (4)$$

U being the Coulomb repulsion parameter. Thus, the model Hamiltonian adopted for this problem is given by

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{\text{ch}}^{\text{imp}} + \mathcal{H}_{\text{ex}}^{\text{imp}} + \mathcal{H}_{\text{Coul}}^{\text{imp}}. \quad (5)$$

B. Equations of motion

In order to calculate the magnetization induced by the local moment $\langle S^x \rangle$ one needs the propagators $G_{ij\sigma}^{dd}(\omega) = \langle \langle d_{i\sigma}; d_{j\sigma}^\dagger \rangle \rangle_\omega$ and $G_{ij\sigma}^{ss}(\omega) = \langle \langle c_{i\sigma}; c_{j\sigma}^\dagger \rangle \rangle_\omega$. (For notation, definitions, and equations of motion see Refs. 7, 14, and 15.) The above propagators are calculated to first order in the exchange couplings, i. e.,

$$G_{ij\sigma}^{\lambda\lambda}(\omega) = G_{ij\sigma}^{\lambda\lambda(0)}(\omega) + G_{ij\sigma}^{\lambda\lambda(1)}(\omega) \quad (\lambda = s \text{ or } d), \quad (6)$$

where the supercripts (0) and (1) indicate the zero-order and the first-order propagators, respectively. Since a Coulomb correlation is present through the term (4) one needs an approximation scheme: In this paper we treat such correlation within the Hartree-Fock picture, which enables us to compare our results with those of Ref. 8.

The equations of motion which determine the propagators are

$$\omega G_{ij\sigma}^{\lambda\lambda}(\omega) = \frac{1}{2\pi} \delta_{ij} \delta_{\lambda\lambda} + \sum_l T_{il}^{(\lambda)} G_{l j\sigma}^{\lambda\lambda}(\omega) + \delta_{i0} V_{dd} G_{0 j\sigma}^{\lambda\lambda}(\omega) + \delta_{i0} \Delta U \langle n_{0-\sigma}^{(d)} \rangle G_{0 j\sigma}^{\lambda\lambda}(\omega) + \delta_{i0} V_{ds} G_{0 j\sigma}^{s\lambda}(\omega) - \sum_l J^{(d)}(\mathbf{R}_i, \mathbf{R}_l) \langle S^x \rangle \sigma G_{l j\sigma}^{\lambda\lambda}(\omega) \quad (7)$$

and

$$G_{i,j\sigma}^{s\lambda}(\omega) = \frac{1}{2\pi} \delta_{ij} \delta_{s\lambda} + \sum_i T_{ii}^{(s)} G_{i,j\sigma}^{s\lambda}(\omega) + \delta_{i0} V_{sd} G_{0,j\sigma}^{d\lambda}(\omega) - \sum_i J^{(s)}(\vec{R}_i, \vec{R}_i) \langle S_i^s \rangle_\sigma G_{i,j\sigma}^{s\lambda}(\omega) \quad (\lambda = s \text{ or } d). \quad (8)$$

It should be noted that Eqs. (7) and (8) are valid to all orders in the perturbations $J^{(d)}$ and $J^{(s)}$. Since we intend to calculate the spin polarization to first order in the exchange parameters, we obtain now the zero-order and the first-order solutions of these equations.

C. Determination of zero-order propagators

Fourier transforming Eqs. (7) and (8) and dropping the exchange terms one obtains equations of motion, in the Bloch representation, for the propagators $G_{\vec{k},\vec{k}';\sigma}^{\lambda\lambda(0)}(\omega)$ and $G_{\vec{k},\vec{k}';\sigma}^{\lambda\beta(0)}(\omega)$ ($\lambda, \beta = s$ or d , $\lambda \neq \beta$). After some algebra one gets for these propagators (where we change variables through $\vec{k}' \rightarrow \vec{k}$ and $\vec{k} \rightarrow \vec{k} + \vec{q}$)

$$G_{\vec{k},\vec{k}';\sigma}^{\lambda\lambda(0)}(\omega) = (2\pi)^{-1} (\omega - \epsilon_{\vec{k}}^{(\lambda)})^{-1} \delta_{\vec{k},\vec{k}'} + (\omega - \epsilon_{\vec{k}+\vec{q}}^{(\lambda)})^{-1} T_{\vec{k},\vec{k}'}^{\lambda\lambda}(\omega) (\omega - \epsilon_{\vec{k}}^{(\lambda)})^{-1}, \quad (9a)$$

$$G_{\vec{k},\vec{k}';\sigma}^{\lambda\beta(0)}(\omega) = (2\pi)^{-1} (\omega - \epsilon_{\vec{k}+\vec{q}}^{(\lambda)})^{-1} T_{\vec{k},\vec{k}'}^{\lambda\beta}(\omega) \times (\omega - \epsilon_{\vec{k}}^{(\beta)})^{-1} \quad (\lambda \neq \beta), \quad (9b)$$

the scattering T matrices being defined as

$$T_{\vec{k},\vec{k}'}^{\lambda\beta}(\omega) = U_{\lambda\beta}^{\sigma}(\omega) / [1 - U_{dd}^{\sigma}(\omega) F_d(\omega)] \quad (\lambda, \beta = s, d), \quad (9c)$$

where

$$F_{\lambda}(\omega) = \sum_{\vec{k}} (\omega - \epsilon_{\vec{k}}^{(\lambda)})^{-1} \quad (\lambda = s \text{ or } d) \quad (9d)$$

and

$$U_{dd}^{\sigma}(\omega) = V_{dd}^{\sigma} + |V_{sd}|^2 F_s(\omega), \quad U_{ss}^{\sigma}(\omega) = |V_{sd}|^2 F_d(\omega), \quad U_{sd}^{\sigma}(\omega) = V_{sd}, \quad U_{ds}^{\sigma}(\omega) = V_{ds}. \quad (9e)$$

In Eqs. (9c) and (9e), $V_{dd}^{\sigma} = V_{dd} + \Delta U \langle n_{0-\sigma}^{(d)} \rangle^{(0)}$ is the localized Hartree-Fock potential which should be determined self-consistently through the propagator $G_{\vec{k},\vec{k}';\sigma}^{dd(0)}(\omega)$. Remembering that, in general,

$$\langle d_{\vec{k}\sigma}^{\dagger} d_{\vec{k}+\vec{q},\sigma} \rangle = \sum_{\vec{k}} \mathcal{F}_{\omega} [G_{\vec{k},\vec{k}';\sigma}^{dd}(\omega)],$$

where \mathcal{F}_{ω} is, as usual,¹⁵

$$\mathcal{F}_{\omega} [G_{\vec{k},\vec{k}';\sigma}(\omega)] = i \int_{-\infty}^{+\infty} d\omega f(\omega) [G_{\vec{k},\vec{k}';\sigma}(\omega + i\epsilon) - G_{\vec{k},\vec{k}';\sigma}(\omega - i\epsilon)], \quad \epsilon \rightarrow 0$$

[$f(\omega)$ being the Fermi-Dirac distribution function], one has

$$V_{dd}^{\sigma} = V_{dd} + \Delta U \sum_{\vec{k},\vec{q}} \mathcal{F}_{\omega} [G_{\vec{k},\vec{k}';\sigma}^{dd(0)}(\omega)]. \quad (10)$$

Equations (9) solve completely the problem of de-

termining the zero-order d - d propagator. It remains, however, the self-consistency problem defined by Eq. (10). Introducing (9a) for $\lambda = d$ in (10) one obtains the self-consistency equation

$$V_{dd}^{\sigma} = V_{dd} + \Delta U \sum_{\vec{k}} f(\epsilon_{\vec{k}}^{(d)}) + \Delta U \mathcal{F}_{\omega} [(F_d(\omega))^2 T_{\vec{k},\vec{k}}^{dd}(\omega, V_{dd}^{\sigma})]. \quad (11)$$

In the following it will be assumed that Eq. (11) shows a paramagnetic solution, namely, $V_{dd}^{\sigma} = V_{dd}^{\dagger} = \tilde{V}_{dd}$. Consequently, in the first-order solution discussed below, the zero-order propagators $G_{\vec{k},\vec{k}';\sigma}^{dd(0)}(\omega)$ and $G_{\vec{k},\vec{k}';\sigma}^{sd(0)}(\omega)$ will be supposed to be spin independent, with $\tilde{V}_{dd} = V_{dd} + \Delta U \langle n_0^{(d)} \rangle^{(0)}$ and spin-independent T matrices. Expressions (9) show that for a given band structure (through the density of states and its Hilbert transform) the zero-order solution is completely determined provided the matrix elements V_{dd} and $|V_{sd}|$ are given. A discussion of approximate procedures to evaluate these parameters is given in Sec. V.

D. Determination of the first-order propagators

Fourier transforming Eqs. (7) and (8) and collecting first-order terms in the exchange parameters one obtains equations of motion for the propagators $G_{\vec{k},\vec{k}';\sigma}^{dd(1)}(\omega)$ and $G_{\vec{k},\vec{k}';\sigma}^{ds(1)}(\omega)$. Denoting by $\Delta n_{0-\sigma}^{(d)}$ the first-order change in occupation number at the impurity site induced by the "external" perturbation $J^{(s)}$ ($\lambda = s, d$) and using the results obtained in Sec. II C for the zero-order propagators, one gets the solution of the coupled system of equations for $G_{\vec{k},\vec{k}';\sigma}^{dd(1)}(\omega)$ and $G_{\vec{k},\vec{k}';\sigma}^{ds(1)}(\omega)$ which gives the first-order correction for the d - d propagator. This propagator is given by the contributions associated with the scattering processes depicted in Figs. 1 and 2 (see also the Appendix B). In Fig. 1 we include the combined scattering associated with the impurity T matrices and with the impurity exchange interaction $J^{(s)}(\vec{k} + \vec{q}, \vec{k})$, whereas in Fig. 2 the combined scattering associated with the change in the Coulomb correlation parameter ΔU and the impurity T matrix is schematically represented.

A convenient approximation is to regard the exchange interaction as being \vec{k}, \vec{k}' independent, so that $J^{(s)}(\vec{k}, \vec{k}') = J^{(s)}$ ($\lambda = s, d$). We expect that such approximation will not destroy the main features of the problem. In this simplified situation, the contribution of the terms described in Fig. 1 to the propagator $G_{\vec{k},\vec{k}';\sigma}^{dd(1)}(\omega)$ is

$$\frac{1}{2\pi} \langle S^s \rangle_{\sigma} \frac{1}{\omega - \epsilon_{\vec{k}+\vec{q}}^{(d)}} \frac{J^{(d)} + J^{(s)} |V_{sd}|^2 [F_{\vec{k}}(\omega)]^2}{[1 - U_{dd}^{\sigma}(\omega) F_d(\omega)]^2} \frac{1}{\omega - \epsilon_{\vec{k}}^{(d)}}. \quad (12a)$$

The terms described in Fig. 2, corresponding to ΔU , assume a simple form when the sums over \vec{k}', \vec{k}'' are evaluated (see Appendix B), namely,

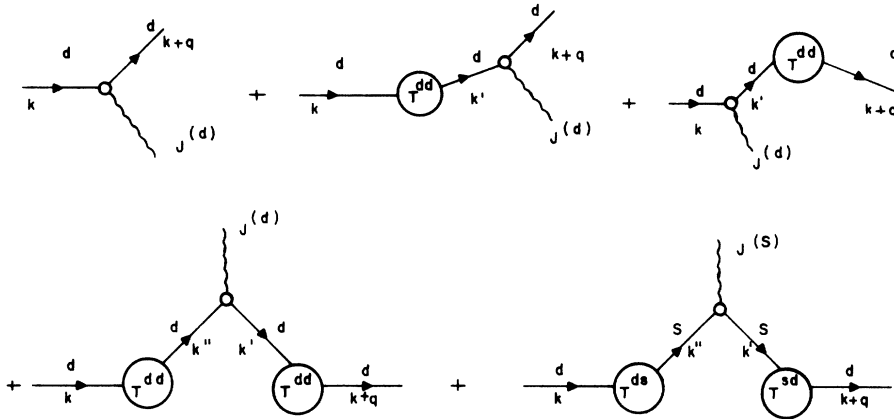


FIG. 1. Scattering processes due to impurity T matrix and exchange couplings associated with the d - d propagator.

$$\frac{1}{2\pi} \frac{1}{\omega - \epsilon_{\vec{k}+\vec{q}}^{(d)}} \frac{\Delta U \Delta n_{\vec{q},-\vec{\sigma}}^{(d)}}{[1 - U_{dd}(\omega) F_d(\omega)]^2} \frac{1}{\omega - \epsilon_{\vec{k}}^{(d)}} \quad (12b)$$

Thus, in the situation where the exchange interaction is taken \vec{k}, \vec{k}' independent, the first-order d - d propagator is

$$G_{\vec{k}+\vec{q}, \vec{k}; \sigma}^{dd(1)}(\omega) = -\frac{1}{2\pi} \frac{1}{\omega - \epsilon_{\vec{k}+\vec{q}}^{(d)}} \frac{\langle S^{\sigma} \rangle \sigma \{ J^{(d)} + J^{(s)} | V_{sd} |^2 [F_d(\omega)]^2 \} - \Delta U \Delta n_{0\sigma}^{(d)}}{[1 - U_{dd}(\omega) F_d(\omega)]^2} \frac{1}{\omega - \epsilon_{\vec{k}}^{(d)}} \quad (13)$$

The first-order s - s propagator is obtained along exactly the same lines. Here we show the final result for the case where the exchange coupling is also assumed to be \vec{k}, \vec{k}' independent:

$$G_{\vec{k}+\vec{q}, \vec{k}; \sigma}^{ss(1)}(\omega) = -\frac{1}{2\pi} \frac{1}{\omega - \epsilon_{\vec{k}+\vec{q}}^{(s)}} \frac{\langle S^{\sigma} \rangle \sigma \{ J^{(s)} [1 - \bar{V}_{dd} F_d(\omega)]^2 + J^{(d)} | V_{sd} |^2 [F_d(\omega)]^2 \} - \Delta U \Delta n_{0-\sigma}^{(d)} | V_{sd} |^2 [F_d(\omega)]^2}{[1 - U_{dd}(\omega) F_d(\omega)]^2} \frac{1}{\omega - \epsilon_{\vec{k}}^{(s)}} \quad (14)$$

III. SPIN POLARIZATION

A. Calculation of d and s magnetizations

From Eqs. (13) and (14) one calculates the first-order change in occupation numbers

$$\Delta n_{\vec{q}}^{\sigma(\lambda)} = \sum_{\vec{k}} \mathcal{F}_{\omega} [G_{\vec{k}+\vec{q}, \vec{k}; \sigma}^{\lambda\lambda(1)}(\omega)] \quad (\lambda = s, d),$$

which yields

$$\Delta n_{\vec{q}}^{\sigma(\lambda)} = \sigma \chi^{\lambda d}(\vec{q}) J^{(d)} \langle S^{\sigma} \rangle + \sigma \chi^{\lambda s}(\vec{q}) J^{(s)} \langle S^{\sigma} \rangle - \chi^{\lambda d}(\vec{q}) \Delta U \Delta n_{0-\sigma}^{(d)} \quad (\lambda = s, d) \quad (15)$$

The explicit forms of the "partial static nonenhanced susceptibilities" $\chi^{\lambda\beta}(\vec{q})$ ($\lambda, \beta = s, d$) are given in Sec. IIIB. The induced λ magnetization is de-

finied, as usual, by $m_{\vec{q}}^{(\lambda)} = \Delta n_{\vec{q}}^{(\lambda)} - \Delta n_{\vec{q}}^{-\sigma(\lambda)}$. From (15), using $\Delta n_{0\sigma}^{(\lambda)} = \sum_{\vec{q}} \Delta n_{\vec{q}}^{\sigma(\lambda)}$, and since $\Delta n_{0\sigma}^{(\lambda)} = -\Delta n_{0-\sigma}^{(\lambda)}$, the self-consistency problem can be easily solved. One gets

$$m_{\vec{q}}^{(\lambda)} = 2\bar{\chi}^{\lambda d}(\vec{q}) J^{(d)} \langle S^{\sigma} \rangle + 2\bar{\chi}^{\lambda s}(\vec{q}) J^{(s)} \langle S^{\sigma} \rangle, \quad (16)$$

where we have defined the "partial static enhanced susceptibilities" $\bar{\chi}^{\lambda\beta}(\vec{q})$ through

$$\bar{\chi}^{\lambda d}(\vec{q}) = \chi^{\lambda d}(\vec{q}) / (1 - \Delta U \chi_0^{dd}) \quad (17a)$$

$$\bar{\chi}^{\lambda s}(\vec{q}) = \chi^{\lambda s}(\vec{q}) + \chi^{\lambda d}(\vec{q}) [\Delta U / (1 - \Delta U \chi_0^{dd})] \chi_0^{ds}, \quad (17b)$$

$\chi_0^{\lambda\beta}$ being

$$\chi_0^{\lambda\beta} = \sum_{\vec{q}} \chi^{\lambda\beta}(\vec{q}) \quad (\lambda, \beta = s, d) \quad (17c)$$

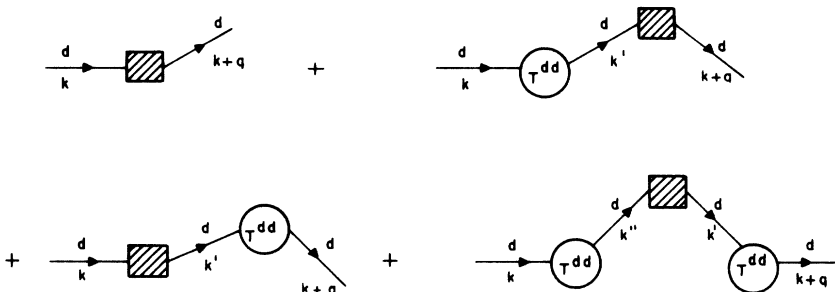


FIG. 2. Scattering processes associated with both impurity T matrix and the change in Coulomb repulsion. The squares represent $\Delta U \Delta n_{0-\sigma}^{(d)}$.

B. Explicit form of nonenhanced susceptibilities

The "partial static nonenhanced susceptibilities" are defined as follows:

$$\chi^{\lambda\lambda}(\vec{q}) = -\frac{1}{2\pi} \sum_{\vec{k}} \mathfrak{F}_{\omega} \times \left[\frac{1}{\omega - \epsilon_{\vec{k}+\vec{q}}^{(\lambda)}} \frac{\delta_{\lambda d} + \delta_{\lambda s} [1 - V_{dd} F_d(\omega)]^2}{[1 - U_{dd}(\omega) F_d(\omega)]^2} \frac{1}{\omega - \epsilon_{\vec{k}}^{(\lambda)}} \right], \quad (18a)$$

$$\chi^{\lambda\beta}(\vec{q}) = -\frac{1}{2\pi} \sum_{\vec{k}} \mathfrak{F}_{\omega} \left[\frac{1}{\omega - \epsilon_{\vec{k}+\vec{q}}^{(\lambda)}} \frac{|V_{sd}|^2 [F_{\beta}(\omega)]^2}{[1 - U_{dd}(\omega) F_d(\omega)]^2} \frac{1}{\omega - \epsilon_{\vec{k}}^{(\lambda)}} \right] \quad (\lambda, \beta = s, d; \lambda \neq \beta). \quad (18b)$$

In order to obtain the explicit form for these susceptibilities, we introduce phase-shifts through

$$F_{\lambda}(\omega) = |F_{\lambda}(\omega)| e^{-i\theta_{\lambda}(\omega)} \quad (\lambda = s, d), \\ X_{dd}(\omega) = 1 - \tilde{V}_{dd} F_d(\omega) = |X_{dd}(\omega)| e^{-i\eta_{dd}(\omega)}, \quad (19) \\ X(\omega) = 1 - U_{dd}(\omega) F_d(\omega) = |X(\omega)| e^{-i\eta(\omega)},$$

where the quantities $|F_{\lambda}(\omega)|$, $|X_{dd}(\omega)|$, $\delta_{\lambda}(\omega)$, $\eta_{dd}(\omega)$, $\eta(\omega)$ are defined in the Appendix A. If one takes into account definitions (19), Eqs. (18) become

$$\chi^{\lambda\beta}(\vec{q}) = \sum_{\vec{k}} \frac{[f_1^{\lambda\beta}(\epsilon_{\vec{k}}^{(\lambda)}) + f_2^{\lambda\beta}(\epsilon_{\vec{k}}^{(\lambda)})] - [f_1^{\lambda\beta}(\epsilon_{\vec{k}+\vec{q}}^{(\lambda)}) + f_2^{\lambda\beta}(\epsilon_{\vec{k}+\vec{q}}^{(\lambda)})]}{\epsilon_{\vec{k}+\vec{q}}^{(\lambda)} - \epsilon_{\vec{k}}^{(\lambda)}} \\ = \sum_{\vec{k}} \frac{\tilde{f}_1^{\lambda\beta}(\epsilon_{\vec{k}}^{(\lambda)}) + \tilde{f}_2^{\lambda\beta}(\epsilon_{\vec{k}+\vec{q}}^{(\lambda)})}{\epsilon_{\vec{k}+\vec{q}}^{(\lambda)} - \epsilon_{\vec{k}}^{(\lambda)}}, \quad (20)$$

where the functions $f_1^{\lambda\beta}(\omega)$ and $f_2^{\lambda\beta}(\omega)$ ($\lambda, \beta = s, d$) are defined in the Appendix C.

An examination of the Eqs. (C1)–(C8) of Appendix C reveals that, in the absence of a perturbative charge potential ($V_{dd} = V_{sd} = 0$), one has

$$f_1^{ds}(\omega) = f_1^{sd}(\omega) = f_2^{sd}(\omega) = f_2^{ds}(\omega) \\ = f_2^{ss}(\omega) = f_2^{dd}(\omega) = 0, \\ f_1^{dd}(\omega) = f_1^{ss}(\omega) = f(\omega),$$

and the partial susceptibilities (18a), (18b), and (20) reduce to

$$\chi^{\lambda\beta}(\vec{q}) = 0 \quad (\lambda, \beta = s, d \text{ and } \lambda \neq \beta), \quad (21a)$$

$$\chi^{\lambda\lambda}(\vec{q}) = \sum_{\vec{k}} \frac{f(\epsilon_{\vec{k}}^{(\lambda)}) - f(\epsilon_{\vec{k}+\vec{q}}^{(\lambda)})}{\epsilon_{\vec{k}+\vec{q}}^{(\lambda)} - \epsilon_{\vec{k}}^{(\lambda)}}, \quad (21b)$$

which is just the classical result for the independent-electron spin polarization due to an external magnetic field. One sees that expressions (20) show the same formal result as the obtained in the pure host case, provided that "new" Fermi distribution functions are introduced. These new distribution functions include scattering effects through phase shifts and the strength of the T matrices.

At this point, some comments are necessary. The "nonenhanced" susceptibilities $\chi^{dd}(\vec{q})$, $\chi^{ds}(\vec{q})$, $\chi^{ss}(\vec{q})$, $\chi^{sd}(\vec{q})$ incorporate, in a natural way, the difference in valence between impurity and host ions, via the phase shifts associated with the charge impurity potential.

From Eqs. (16) one sees that, even in presence of Coulomb correlations at the impurity site, the d and s magnetizations can be written in terms of "partial susceptibilities." Equations (17) show clearly the effects of ΔU : The susceptibilities associated with the response to the local moment coupling $J^{(d)}$ are enhanced or reduced, depending on the sign of ΔU , by the factor $(1 - \Delta U \chi_0^{dd})^{-1}$, and the susceptibilities associated with $J^{(s)}$ coupling are corrected by adding (or subtracting) a " ΔU scattering factor."

Now, it is useful to recall the case of independent bands (neglecting the impurity-induced mixing). The susceptibilities $\chi^{ds}(\vec{q})$ and $\chi^{sd}(\vec{q})$ vanish, and from Eqs. (16) and (17) one gets

$$m_q^{(d)} = [\chi^{dd}(\vec{q}) / (1 - \Delta U \chi_0^{dd})] 2J^{(d)} \langle S^z \rangle \quad (22)$$

and

$$m_q^{(s)} = \chi^{ss}(\vec{q}) 2J^{(s)} \langle S^z \rangle. \quad (23)$$

Expression (22) for the d magnetization may be compared with the susceptibilities obtained by Mills and Lederer⁸ for the case of a single d band in the presence of externally applied frequency ω and wave-vector- \vec{q} -dependent magnetic field. Besides the field, these authors include at the impurity site a charge potential and the effect of ΔU [see Eq. (11) of Ref. 8]. Now, in the static limit ($\omega = 0$) of Ref. 8, we recall that a \vec{k}, \vec{k}' -independent exchange coupling can be interpreted as being an external static magnetic field acting only at the origin. The fact that the field acts only at the origin amounts to considering an external field of the form $h_0 \sum_{\vec{r}_i} e^{-i\vec{q} \cdot \vec{R}_i}$. Then, summing over the values of the wave vector \vec{q}' , considered in Ref. 8, one obtains a formally identical result to ours [cf. Eq. (22)], with $h_0 = J^{(d)} \langle S^z \rangle$.

This similarity is to be expected since both approaches are linear-response calculations, ours being a static one, which can be easily generalized to a dynamic one within the random-phase approximation. Recall that in our case, the weak "external" field is the impurity spin s - f and d - f exchange fields.

Now we make some comments about the correlations in the host. The adopted approximation, neglecting all Coulomb correlations in the host, excludes strongly exchange-enhanced hosts, like Pd metal, for instance, where the Stoner criterion is nearly satisfied. The calculation including the intra-atomic Coulomb correlations in the host can only be obtained on formal grounds in terms of a

power series under the assumption of a local screening.¹⁶

IV. SPIN POLARIZATION AT IMPURITY SITE

In this section we describe how to complement the results obtained by Blandin and Campbell.⁶ We recall that in their paper the magnetic moments were assumed to be at least at a distance \bar{R}_0 from the charge impurity center.

On the other hand, we consider throughout this paper the limit $\bar{R}_0 = 0$ for the magnetic impurity, i. e., charge potential source of scattering and local moment located at the same site. As an implication of our approach, it is possible to evaluate the self-polarization hyperfine field induced by the magnetic rare-earth atom embedded in the transition-metal host. This particular situation simplifies considerably the calculations as compared to the general formulas (18) and (20), which are appropriate to the calculation of the long-range polarization (to be used, for instance, in indirect g -shift calculations). A similar simplification occurs in the discussion of the spin disorder resistivity associated with the magnetic rare-earth atom.¹⁰

To derive the self-polarization field one just needs to sum up over \bar{q} expressions (18). For example, in the case of the "nonenhanced" d - d susceptibility, one has

$$\begin{aligned} \chi^{dd}(0) &= \chi_0^{dd} = \sum_{\bar{q}} \chi^{dd}(\bar{q}) \\ &= -\frac{1}{2\pi} \mathcal{F}_\omega \left[\frac{[F_d(\omega)]^2}{[1 - \bar{V}_{dd} F_d(\omega) - |V_{sd}|^2 F_s(\omega) F_d(\omega)]^2} \right]. \end{aligned} \quad (24)$$

Now, using the definitions of Appendix A, one obtains

$$\chi^{dd}(0) = \frac{1}{\pi} \int \frac{|F_d(\omega)|^2}{|X(\omega)|^2} \sin[2\eta(\omega) - 2\delta_d(\omega)] f(\omega) d\omega. \quad (25)$$

So, the "enhanced" d - d susceptibility at the origin is

$$\bar{\chi}^{dd}(0) = \chi^{dd}(0) / [1 - \Delta U \chi^{dd}(0)]. \quad (26)$$

Quite similarly, one derives the other local partial static susceptibilities, the magnetizations at the origin being given by

$$\begin{aligned} m^{(\lambda)}(0) &= 2\bar{\chi}^{\lambda\lambda}(0) J^{(\lambda)} \langle S^x \rangle + 2\bar{\chi}^{\lambda\beta}(0) J^{(\beta)} \langle S^y \rangle \\ &\quad (\lambda, \beta = s, d; \lambda \neq \beta). \end{aligned} \quad (27)$$

It should be emphasized that for $T = 0^\circ\text{K}$ [where $f(\omega) = 1$ and $\omega < \epsilon_F$], expression (25) can be easily computed given the density of states and the parameters V_{dd} , $|V_{sd}|$ (see Sec. V), and ΔU . One expects from expression (25) through the term $\sin[2\eta(\omega) - 2\delta_d(\omega)]$ a possible change of sign of the magnetic response. The detailed study of this particular problem will appear soon¹⁷ and will not

be discussed further in this paper. The only thing we want to suggest is that the result obtained in Ref. 6 may be extended to $\bar{R}_0 = 0$ and that the changes in sign are a general result of combined spin and charge potentials.^{6,21}

V. ESTIMATE OF IMPURITY POTENTIAL PARAMETERS (V_{dd} AND $|V_{sd}|$)

The results of Sec. III B and the expressions for the phase shifts (see Appendix A) show that for given matrix elements V_{dd} and $|V_{sd}|$ the new Fermi functions f_1 and f_2 are completely specified by the knowledge of the band structure through $\rho_\lambda(\omega)$ ($\lambda = s, d$) and their Hilbert transforms.

The explicit determination of the matrix elements V_{dd} and V_{sd} can be made under some simplifying hypothesis.

A first alternative consists in assuming that screening satisfies the Friedel sum rule¹⁸ neglecting the contribution of s - d mixing to the screening. The usual result is then

$$\Delta Z = -\frac{1}{\pi} \sum_{\sigma} \arctan \frac{\pi V_{dd}^{\sigma} \rho_d(\epsilon_F)}{1 - V_{dd}^{\sigma} F_d^R(\epsilon_F)}, \quad (28)$$

where ΔZ is the extra charge introduced by the impurity, $\rho_d(\omega)$ and $F_d^R(\omega)$ being, respectively, the pure host d -band density of states and its Hilbert transform (cf. Appendix A), and ϵ_F is the Fermi energy. Expression (28) together with (11), where s - d mixing is consistently neglected also, determines completely the matrix elements V_{dd}^{σ} . One should note that for $T = 0^\circ\text{K}$ expression (11) can be cast in a more simple form [neglecting $|V_{sd}|^2$ as in Eq. (28)],

$$\begin{aligned} V_{dd}^{\sigma} &= V_{dd} + \Delta U n_h + \Delta U \int_0^{\epsilon_F} \rho_d(\omega) d\omega \{ [1 - V_{dd}^{\sigma} F_d^R(\omega)]^2 \\ &\quad + [\pi V_{dd}^{\sigma} \rho_d(\omega)]^2 \}^{-1/2}, \end{aligned} \quad (29)$$

where $n_h = \sum_{\mathbf{k}} f(\epsilon_{\mathbf{k}}^{(\lambda)})$ is the number of electrons in the host metal. Equations (28) and (29) show that V_{dd}^{σ} is completely specified by the band structure [through $\rho_d(\omega)$], the charge difference ΔZ , and the Coulomb energy parameter ΔU . As assumed throughout the calculation we suppose that the solution is nonmagnetic, i. e., $V_{dd}^{\sigma} = \bar{V}_{dd}$. It remains to estimate the mixing matrix elements $|V_{sd}|$, which in this simplified picture act only as a source of scattering between s and d states and as the principal source of scattering for the s electrons. It may be shown, by calculating the imaginary part of the scattering matrix $T^{ss}(\omega)$, $|V_{sd}|^2$, that the residual resistivity ΔR for nonmagnetic rare-earth impurities is proportional to^{9,10}

$$\Delta R \propto \frac{|V_{sd}|^2 \pi \rho_d(\epsilon_F)}{[1 - \bar{V}_{dd} F_d^R(\epsilon_F)]^2 + [\pi \bar{V}_{dd} \rho_d(\epsilon_F)]^2}. \quad (30)$$

Then, using resistivity measurements for these

impurities (e.g., Lu) diluted in transitionlike metals one can obtain ΔR . So, from (30), together with the previously obtain value of V_{dd} , one determines $|V_{sd}|^2$.

A second alternative would be, instead of giving primary importance to the screening sum rule, to adopt the procedure suggested by Hayakawa¹⁹ and to construct the impurity potential starting from potentials corresponding to different atomic configurations. (We are grateful to Dr. J. A. B. Carvalho for very useful discussions concerning this point.) Following Ref. 19 one has

$$V_{\text{imp}} = a V_1 [n' d^{n'+\Delta Z} (n'+1) s^{-1}] + b V_2 [n' d^{n'+\Delta Z-1} (n'+1) s^{-1}], \quad (31)$$

where V_1 and V_2 are the atomic potentials corresponding to d configurations of $n + \Delta Z$ or $n + \Delta Z - 1$ electrons. In (31) n' may assume the values 3, 4, 5 according to the transition series, n taking on values between 1 and 10. The first term of (31) corresponds to perfect screening at the impurity site (the number of d electrons changing by ΔZ) and the second one to an excess of one charge in respect to perfect screening. Since one has a change in d -occupation number $\sum_{\sigma} \Delta n_{0\sigma}^{(0)}$ the coefficients a and b must satisfy

$$a \Delta Z + b(\Delta Z - 1) = \sum_{\sigma} \Delta n_{0\sigma}^{(0)} (V_{dd}^{\sigma} | V_{sd} |), \quad (32a)$$

and naturally

$$a + b = 1. \quad (32b)$$

Equations (31) and (32) define a self-consistency problem, determining the amount of configuration admixture at the impurity site. In this model the relevant matrix elements are obtained as a linear combination of matrix elements associated to the potentials V_1 and V_2 which are known from atomic tables. From (31) one has

$$\langle d | V_{\text{imp}} - V_{\text{host}} | d \rangle = a \delta V_{dd}^{(1)} + b \delta V_{dd}^{(2)} = V_{dd}, \quad (33a)$$

$$\langle s | V_{\text{imp}} - V_{\text{host}} | d \rangle = a \delta V_{sd}^{(1)} + b \delta V_{sd}^{(2)} = V_{sd}, \quad (33b)$$

where V_{host} is the potential used in the construction of the host band structure. It should be noted that in the model adopted here the s - d mixing matrix elements of these potentials are obtained by computing matrix elements between plane waves \mathbf{k} and d states and, after that, averaging over the wave vectors \mathbf{k} up to the Fermi level. On the other hand, from Eqs. (32) it follows that

$$a = -\Delta Z + 1 + \sum_{\sigma} \Delta n_{0\sigma}^{(0)} (V_{dd}^{\sigma} | V_{sd} |).$$

So, V_{dd} is written

$$V_{dd} = \delta V_{dd}^{(2)} - (\Delta Z - 1) (\delta V_{dd}^{(1)} - \delta V_{dd}^{(2)}) + (\delta V_{dd}^{(1)} - \delta V_{dd}^{(2)}) \times \sum_{\sigma} \Delta n_{0\sigma}^{(0)} (V_{dd}^{\sigma} | V_{sd} |), \quad (34)$$

and for V_{sd} one gets

$$V_{sd} = \delta V_{sd}^{(2)} - (\Delta Z - 1) (\delta V_{sd}^{(1)} - \delta V_{sd}^{(2)}) + (\delta V_{sd}^{(1)} - \delta V_{sd}^{(2)}) \times \sum_{\sigma} \Delta n_{0\sigma}^{(0)} (V_{sd}^{\sigma} | V_{sd} |). \quad (35)$$

Hence, according to Eq. (11), V_{dd}^{σ} turns out to be

$$V_{dd}^{\sigma} = V_{dd} + \Delta U (n_h + \Delta n_{0-\sigma}^{(0)}) = \delta V_{dd}^{(2)} - (\Delta Z - 1) (\delta V_{dd}^{(1)} - \delta V_{dd}^{(2)}) + (\delta V_{dd}^{(1)} - \delta V_{dd}^{(2)}) \times \sum_{\sigma} \Delta n_{0\sigma}^{(0)} (V_{dd}^{\sigma} | V_{sd} |) + \Delta U (n_h + \Delta n_{0-\sigma}^{(0)}). \quad (36)$$

From Eqs. (35) and (36) it is clear that the matrix elements $|V_{sd}|$ and V_{dd}^{σ} are determined in terms of $\delta V^{(1)}$, $\delta V^{(2)}$, ΔZ , and $\Delta n_{0\sigma}^{(0)} (V_{dd}^{\sigma} | V_{sd} |)$. Since $\delta V^{(1)}$ and $\delta V^{(2)}$ are known from atomic tables, to complete the procedure one needs an explicit expression for $\Delta n_{0\sigma}^{(0)}$ in terms of the matrix elements V_{dd}^{σ} , V_{sd} and the band structure of the host.

Recalling that

$$\Delta n_{0\sigma}^{(0)} = \mathcal{F}_{\omega} [(F_d(\omega))^2 T_{\sigma}^{dd}(\omega, V_{dd}^{\sigma} | V_{sd} |^2)],$$

one obtains

$$\Delta n_{0\sigma}^{(0)} \cong \int_0^{\epsilon_F} d\omega \rho_d(\omega) \left(\frac{1 + |V_{sd}|^2 \{ \pi^2 \rho_s(\omega) \rho_d(\omega) + [F_d^R(\omega)]^2 \rho_s(\omega) / \rho_d(\omega) \}}{D(\omega)} - 1 \right), \quad (37a)$$

where

$$D(\omega) = \{ 1 - V_{dd}^{\sigma} F_d^R(\omega) - |V_{sd}|^2 [F_d^R(\omega) F_s^R(\omega) - \pi^2 \rho_d(\omega) \rho_s(\omega)] \}^2 + \{ \pi V_{dd}^{\sigma} \rho_d(\omega) + |V_{sd}|^2 [\rho_d(\omega) F_s^R(\omega) + \rho_s(\omega) F_d^R(\omega)] \}^2, \quad (37b)$$

and so it is possible to determine self-consistently the potentials V_{dd}^{σ} and $|V_{sd}|$. Again it is assumed that the solution is nonmagnetic, i.e., $V_{dd}^{\sigma} = \bar{V}_{dd}$. Once determined, from one method or the other, the values obtained for V_{dd} and $|V_{sd}|$ can be used in the explicit calculation of the phase shifts and partial susceptibilities.

VI. FINAL REMARKS

From the model described in the text is clear that the rare-earth impurity introduced in the transition host acts in two ways:

(i) The simplest effect is that the f level (supposed to lie below the conduction s - d bands) pro-

vides only a source of one-electron spin-dependent potential via the exchange interactions s - f and d - f . Its isolated effect has been extensively discussed in the literature¹⁻³ and extensions to include hybridization (s - d host hybridization) have been made.^{4,20}

(ii) The valence state of the usual rare earths (trivalent in general) introduces a new feature of the impurity, since the potential associated with the charge difference provides a new source of scattering. In the case discussed here, primary importance is given to the nature of the host, namely, the existence of s - d bands.

The effect of potential scattering associated with the rare-earth impurity in ferromagnetic transition metals has been invoked in a previous work.²¹ There, it was shown that potential scattering associated with the rare-earth impurity may drastically modify the behavior of the d magnetic moment, thus coupling the rare earth's f moment antiparallel to the host magnetization.

Another aspect of the combined effect of spin and charge potentials was discussed within a one-band model by Blackman and Elliot in the context of the calculation of spin-disorder resistivity²² and Ruderman-Kittel-Kasuya-Yosida interaction.²³ In these works (and their extension to describe s - d bands and hybridization effects¹⁰) the effect of potential scattering is also included in the phase shifts, their behavior as a function of the energy determining the net effect in these quantities of the impurity charge scattering.

The recent work of Blandin and Campbell⁶ involves also the combined effect of charge potential scattering and spin-dependent potential, in the context of the calculation of the spin polarization. Note that the above authors⁶ also treat the exchange interaction to first order in perturbation theory. Their work, assuming a nonmagnetic impurity at the origin and magnetic moments far apart from it by at least a distance \bar{R}_0 , has for its main result that the usual spin polarization includes a phase shift determined by the strength of the one-electron local perturbation.

Our calculation above, although involving more complicated steps, may explore a typical feature of narrow d bands. In fact, besides providing the limit $\bar{R}_0 = 0$ of Ref. 6 (cf. Sec. IV), it is known¹⁸ that the behavior of phase shifts (defining the impurity response, within the Hartree-Fock approach) depends strongly on the details of the d density of states,¹⁸ which in our case may assume arbitrary shape. The price to be paid for this generality in the band structure is the more complex nature of the expression giving the spin polarization for these two-band systems. However, the limiting situation of Sec. IV of the polarization at the impurity site, provides a simple expression which

can be easily evaluated numerically, even in presence of the complex band structure of the transition metal.

Other quantities, e.g., the spin-disorder resistivity and the Ruderman-Kittel-Kasuya-Yosida interaction as shown in Refs. 22, 23, and 10, have a more simple dependence on the phase shifts than the spin polarization does.

As discussed in Sec. III, whence the potential matrix elements are obtained, the computation of the phase shifts gives directly the effect of the impurity charge scattering on the spin polarization. In the long-range spin-polarization case [cf. formulas (18) and (20)], since phase shifts appear as giving rise to "modified Fermi functions," the computation of the partial susceptibilities requires a quite delicate numerical analysis. In fact, if one is interested in obtaining the effects of a d -band structure (virtual bound states, peaks, etc.), they appear naturally in our formalism via the phase shifts, but in a much more complex form through these modified Fermi functions (cf. Appendix C), thus changing the usual behavior of a magnetic response problem, which is always given in terms of common Fermi functions. So, the procedures introduced by Diamond²⁴ and Lipton and Jacobs²⁵ should be extended to include new functions which may assume other values than 0 or 1. Hence, besides the problem of investigation the role in long-range spin-polarization of the details of the band structure, expressions (C1)-(C8) add the problem of extending available numerical techniques to evaluate magnetic response functions.

The best way to discuss the role of the band structure in resonant scattering (virtual bound states), peaks, and so on, is to adopt a realistic band structure and calculate the susceptibilities involved. By changing in the band structure the position of the Fermi level, in order to scan the neighborhood of the top of the band, the regions of narrow peaks, etc., the role of these details may be discussed properly. Such an analysis, however, is beyond the scope of this article.

As far as the experimental situation is concerned, we would like to point out some possible uses of our calculations. Besides the determination of the residual resistivity of transition alloys with nonmagnetic rare earths, which could provide a way of estimating $|V_{sd}|$ (as discussed in Sec. V), measures of indirect g shift could be of interest. This class of experiments would measure the indirect g shifts, keeping fixed the "resonant" (e.g., Gd) and "nonresonant" (e.g., Tb) rare-earth impurity but changing the transition host, in order to vary the nature of the host band structure. Systems like NiRh alloys, for instance, with rare-earth impurities, by changing the amount of Ni and Rh would provide a changing d -electron structure.

A measure of indirect g shift as a function of concentration could exhibit experimental evidence for the effect of changing the d -band structure on the spin polarization

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APPENDIX A: PHASE-SHIFT PARAMETERS

Taking into account definition (9d), for $\omega \pm i\epsilon$ in the limit $\epsilon \rightarrow 0$, one has real and imaginary parts. Hence

$$F_\lambda(\omega \pm i\epsilon) = F_\lambda^R(\omega) \mp i F_\lambda^I(\omega) \quad (\lambda = s, d), \quad (\text{A1})$$

where

$$F_\lambda^R(\omega) = \mathcal{P} \sum_{\mathbf{k}} \frac{1}{\omega - \epsilon_{\mathbf{k}}^{(\lambda)}} F_\lambda^I(\omega) = \pi \rho_\lambda(\omega), \quad (\text{A2})$$

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

$$F_\lambda(\omega \pm i\epsilon) = |F_\lambda(\omega)| e^{\mp i\delta_\lambda(\omega)}, \quad (\text{A3})$$

where

$$|F_\lambda(\omega)| = \{[F_\lambda^R(\omega)]^2 + [F_\lambda^I(\omega)]^2\}^{1/2}, \quad (\text{A4})$$

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

It is clear that

$$F_s(\omega \pm i\epsilon) F_d(\omega \pm i\epsilon) = |F_s(\omega)| |F_d(\omega)| e^{\mp i[\delta_s(\omega) + \delta_d(\omega)]}. \quad (\text{A5})$$

Similarly,

$$1 - \tilde{V}_{dd} F_d(\omega \pm i\epsilon) = |1 - \tilde{V}_{dd} F_d(\omega)| e^{\mp i\eta_{dd}(\omega)} \\ = |X_{dd}^{(\omega)}| e^{-i\eta_{dd}(\omega)}, \quad (\text{A6})$$

where

$$|X_{dd}(\omega)| = \{[1 - \tilde{V}_{dd} F_d^R(\omega)]^2 + [\tilde{V}_{dd} F_d^I(\omega)]^2\}^{1/2}, \\ \cos \eta_{dd}(\omega) = [1 - \tilde{V}_{dd} F_d^R(\omega)] / |1 - \tilde{V}_{dd} F_d(\omega)|, \quad (\text{A7})$$

$$\sin \eta_{dd}(\omega) = -\tilde{V}_{dd} F_d^I(\omega) / |1 - \tilde{V}_{dd} F_d(\omega)|,$$

and finally

$$1 - \tilde{V}_{dd} F_d(\omega \pm i\epsilon) - |V_{sd}|^2 F_s(\omega \pm i\epsilon) F_d(\omega \pm i\epsilon) \\ = |X(\omega)| e^{\mp i\eta(\omega)}, \quad (\text{A8})$$

where

$$|X(\omega)| = \{[1 - \tilde{V}_{dd} F_d^R(\omega) - |V_{sd}|^2 [F_d^R(\omega) F_s^R(\omega) - F_d^I(\omega) F_s^I(\omega)]]^2 + [\tilde{V}_{dd} F_d^I(\omega) - |V_{sd}|^2 [F_d^R(\omega) F_s^I(\omega) + F_d^I(\omega) F_s^R(\omega)]]^2\}^{1/2}, \quad (\text{A9})$$

$$\cos \eta(\omega) = \frac{1 - \tilde{V}_{dd} F_d^R(\omega) - |V_{sd}|^2 [F_d^R(\omega) F_s^R(\omega) - F_d^I(\omega) F_s^I(\omega)]}{|X(\omega)|}, \quad (\text{A10})$$

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

APPENDIX B: GENERAL EXPRESSION FOR PROPAGATOR $G_{\mathbf{k}+\mathbf{q},\mathbf{k};\sigma}^{dd(1)}(\omega)$

In this appendix, we exhibit the final result for the first-order correction in the one-electron \bar{a} - d propagator, when the full \mathbf{k}, \mathbf{k}' dependence in the exchange couplings is included. One has

$$G_{\mathbf{k}+\mathbf{q},\mathbf{k};\sigma}^{dd(1)}(\omega) = -\frac{1}{2\pi} \frac{1}{\omega - \epsilon_{\mathbf{k}+\mathbf{q}}^{(d)}} \left(J^{(d)}(\mathbf{k} + \mathbf{q}, \mathbf{k}) \langle S^\sigma \rangle_\sigma + \sum_{\mathbf{k}'} J^{(d)}(\mathbf{k} + \mathbf{q}, \mathbf{k}') \langle S^\sigma \rangle_\sigma \frac{1}{\omega - \epsilon_{\mathbf{k}'}^{(d)}} T^{dd}(\omega) + T^{dd}(\omega) \sum_{\mathbf{k}'} \frac{1}{\omega - \epsilon_{\mathbf{k}'}^{(d)}} J^{(d)}(\mathbf{k}', \mathbf{k}) \right. \\ \times \langle S^\sigma \rangle_\sigma + T^{dd}(\omega) \sum_{\mathbf{k}', \mathbf{k}''} \frac{1}{\omega - \epsilon_{\mathbf{k}'}^{(d)}} J^{(d)}(\mathbf{k}', \mathbf{k}'') \langle S^\sigma \rangle_\sigma \frac{1}{\omega - \epsilon_{\mathbf{k}''}^{(d)}} T^{dd}(\omega) + T^{ds}(\omega) \sum_{\mathbf{k}', \mathbf{k}''} \frac{1}{\omega - \epsilon_{\mathbf{k}'}^{(s)}} J^{(s)}(\mathbf{k}', \mathbf{k}'') \langle S^\sigma \rangle_\sigma \frac{1}{\omega - \epsilon_{\mathbf{k}''}^{(s)}} \\ \left. \times T^{sd}(\omega) \right) \frac{1}{\omega - \epsilon_{\mathbf{k}}^{(d)}} + \frac{1}{2\pi} \frac{1}{\omega - \epsilon_{\mathbf{k}+\mathbf{q}}^{(d)}} \left(\Delta U \Delta n_{0-\sigma}^{(d)} + \Delta U \Delta n_{0-\sigma}^{(d)} \sum_{\mathbf{k}'} \frac{1}{\omega - \epsilon_{\mathbf{k}'}^{(d)}} T^{dd}(\omega) + T^{dd}(\omega) \sum_{\mathbf{k}'} \frac{1}{\omega - \epsilon_{\mathbf{k}'}^{(d)}} \Delta U \Delta n_{0-\sigma}^{(d)} \right. \\ \left. + T^{dd}(\omega) \sum_{\mathbf{k}', \mathbf{k}''} \frac{1}{\omega - \epsilon_{\mathbf{k}'}^{(d)}} \Delta U \Delta n_{0-\sigma}^{(d)} \frac{1}{\omega - \epsilon_{\mathbf{k}''}^{(d)}} T^{dd}(\omega) \right) \frac{1}{\omega - \epsilon_{\mathbf{k}}^{(d)}}. \quad (\text{B1})$$

This lengthy expression is to be compared with the simplicity of the result of the text [cf. Eq. (13)], thus emphasizing the complexities introduced in the self-consistency problem by the \mathbf{k}, \mathbf{k}' dependence.

APPENDIX C: DEFINITION OF FUNCTIONS $f_1^{\lambda\beta}(\omega)$ AND $f_2^{\lambda\beta}(\omega)$ ($\lambda, \beta = s, d$)

$$f_1^{dd}(\omega) = |X(\omega)|^{-2} \cos[2\eta(\omega)] f(\omega), \quad (\text{C1})$$

$$f_1^{ds}(\omega) = |V_{sd}|^2 |F_s(\omega)/X(\omega)|^2 \cos[2\eta(\omega) - 2\delta_s(\omega)] f(\omega), \quad (\text{C2})$$

$$f_2^{da}(\omega) = \frac{1}{\pi} \mathcal{P} \int \frac{d\omega' f(\omega') |X(\omega')|^{-2} \sin[2\eta(\omega')]}{\omega' - \omega}, \quad (C3)$$

$$f_2^{ds}(\omega) = \frac{1}{\pi} \mathcal{P} \int \frac{d\omega' f(\omega') |V_{sd}|^2 |F_s(\omega')/X(\omega')|^2 \sin[2\eta(\omega') - 2\delta_s(\omega')]}{\omega' - \omega}, \quad (C4)$$

$$f_1^{ss}(\omega) = |X_{da}(\omega)/X(\omega)|^2 \cos[2\eta(\omega) - 2\eta_{da}(\omega)] f(\omega), \quad (C5)$$

$$f_1^{sd}(\omega) = |V_{sd}|^2 |F_d(\omega)/X(\omega)|^2 \cos[2\eta(\omega) - 2\delta_d(\omega)] f(\omega), \quad (C6)$$

$$f_2^{ss}(\omega) = \frac{1}{\pi} \mathcal{P} \int \frac{d\omega' f(\omega') |X_{da}(\omega')/X(\omega')|^2 \sin[2\eta(\omega') - 2\eta_{da}(\omega')]}{\omega' - \omega}, \quad (C7)$$

$$f_2^{sd}(\omega) = \frac{1}{\pi} \mathcal{P} \int \frac{d\omega' f(\omega') |V_{sd}|^2 |F_d(\omega')/X(\omega')|^2 \sin[2\eta(\omega') - 2\delta_d(\omega')]}{\omega' - \omega}, \quad (C8)$$

\mathcal{P} denoting Cauchy's principal value.

Note added in proof: The second alternative estimate of the impurity parameters can be improved (screening condition) using the methods of Ref. 13.

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