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REMARKS ON THE EFFECT OF s-d MIXING IN THE SPIN POLARIZATION;
HARTREE-FOCK APPROACH

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REMARKS ON THE EFFECT OF s-d MIXING IN THE SPIN POLARIZATION;
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INTRODUCTION

The role of intraband exchange enhancement and of the k, k' dependence of the exchange integral among itinerant and localized spins has been discussed recently in several works [1], [2], [3]. The role of intraband exchange enhancement in metals has been discussed in connection to indirect g-shifts [1], spin lattice relaxation [2], etc. On the other hand, the discussion of the details of the k, k' dependence of the coupling among itinerant and localized (d or f) has been the subject of several papers [3] usually in the context of the calculation of the spin polarization (necessary to calculate hyperfine fields, in particular the self-polarization field).

In recent years, the role of d-bands in rare-earth metals and alloys,

in particular its connection to some controversial signs of the exchange parameter (as determined by E.S.R. measurements) has been the subject of much interest [4], [5], [6]. It has been suggested that s-d mixing effects play an important role in defining the sign of the effective exchange acting on s and d electrons in rare-earths and intermetallic systems [5], [6], [7]. Using a rather phenomenological approach, Gomes et al [5], following the model of Coles [4] were able to discuss negative signs of the exchange couplings in Gd and some intermetallic compounds. It is the purpose of this paper to extend the calculation of Giovannini et al [1] to include the k, k' dependence of the exchange coupling and the existence of hybridized s and d bands. This picture seems adequate to describe the situation encountered in rare-earth metals, alloys and intermetallics where band calculations show the existence of a transition of a transition metal like band structure. We conserve the Hartree-Fock approximation used in [1] in discussing intra d-band correlations, the opposite limit of strong correlations being discussed in another paper [8]. The result of the calculation is an explicit expression for the effective exchange couplings in terms of the "bare" exchange parameters $J^{(s)}(k, k')$, $J^{(d)}(k, k')$ and of the band structure (through the mixing matrix elements and the susceptibilities). These results are compared to the phenomenological ones obtained in [5]. Finally the methods that should be used for numerical computation are briefly indicated.

II - FORMULATION OF THE PROBLEM

We describe the conduction states as s-d hybridized d and s bands; in the Wannier representation:

$$H_0 = \sum_{i,j,\sigma} T_{ij}^{(s)} c_{i\sigma}^+ c_{j\sigma} + \sum_{i,j,\sigma} T_{ij}^{(d)} d_{i\sigma}^+ d_{j\sigma} + \sum_{i,j,\sigma} \{ V_{sd}(R_i - R_j) c_{i\sigma}^+ d_{j\sigma} + V_{ds}(R_i - R_j) d_{i\sigma}^+ c_{j\sigma} \} \quad (1)$$

where k dependent matrix elements are assumed for the s - d mixing, namely:

$$V_{sd}(R_i - R_j) = \sum_k V_{sd}(k) e^{ik(R_i - R_j)}$$

The impurity spin is coupled to the conduction states through:

$$H_{imp} = \sum_{i,j,\sigma} J^{(s)}(R_i, R_j) \langle S^Z \rangle_{\sigma} c_i^{\dagger} c_j + \sum_{i,j,\sigma} J^{(d)}(R_i - R_j) \langle S^Z \rangle_{\sigma} d_{i\sigma}^{\dagger} d_{j\sigma} \quad (2)$$

Finally it is assumed that Coulomb interaction exists among d -electrons and this effect is described through:

$$H_{coul} = I \sum_i n_{i\uparrow}^{(d)} n_{i\downarrow}^{(d)} \quad (3)$$

The complete hamiltonian is then:

$$H = H_0 + H_{coul} + H_{imp} \quad (4)$$

In order to calculate the spin polarization associated to $\langle S^Z \rangle$ one needs the propagators $G_{ij}^{SS}(\omega) = \langle\langle c_{i\sigma}; c_{j\sigma}^{\dagger} \rangle\rangle_{\omega}$ and $G_{ij}^{dd}(\omega) = \langle\langle d_{i\sigma}; d_{j\sigma}^{\dagger} \rangle\rangle$. These propagators are calculated to first order in the exchange parameters (linear response). Due to the existence of the two-body term (3) some type of approximation is needed in order to treat the equations of motion. Here we choose the Hartree-Fock approximation in order to follow as closely as possible

the work of Giovannini et al. [1].

a) Determination of the equations of motion

Using the Hamiltonian (4) one gets:

$$\begin{aligned} \omega G_{ij}^{SS}(\omega) = & \frac{\delta_{ij}}{2\pi} + \sum_{\ell} T_{i\ell}^{(s)} G_{\ell j}^{SS}(\omega) + \sum_{\ell} V_{sd}(R_i - R_{\ell}) G_{\ell j}^{ds}(\omega) \\ & + \langle S^Z \rangle_{\sigma} \sum_{\ell} J_{\ell}^{(s)}(R_i, R_{\ell}) G_{\ell j}^{SS} \end{aligned} \quad (5)$$

The propagator $G_{ij}^{ds}(\omega)$ satisfies in the Hartree-Fock approximation:

$$\begin{aligned} \omega G_{ij}^{ds}(\omega) = & \sum_{\ell} T_{i\ell}^{(d)} G_{\ell j}^{ds}(\omega) + I \langle \eta_{i-\sigma} \rangle G_{ij}^{ds}(\omega) + \sum_{\ell} V_{ds}(R_i - R_{\ell}) G_{\ell j}^{SS}(\omega) \\ & + \langle S^Z \rangle_{\sigma} \sum_{\ell} J_{\ell}^{(d)}(R_i, R_{\ell}) G_{\ell j}^{ds}(\omega) \end{aligned} \quad (6)$$

The coupled equations (5) and (6) determine completely the propagator $G_{ij}^{SS}(\omega)$.

Now we proceed determining the propagators $G_{ij}^{dd}(\omega)$; one has:

$$\begin{aligned} \omega G_{ij}^{dd}(\omega) = & \frac{1}{2\pi} \delta_{ij} + \sum_{\ell} T_{i\ell}^{(d)} G_{\ell j}^{dd}(\omega) + I \langle \eta_{i-\sigma}^{(d)} \rangle G_{ij}^{dd}(\omega) + \sum_{\ell} V_{ds}(R_i - R_{\ell}) G_{\ell j}^{sd}(\omega) \\ & + \langle S^Z \rangle_{\sigma} \sum_{\ell} J_{\ell}^{(d)}(R_i, R_{\ell}) G_{\ell j}^{dd}(\omega) \end{aligned} \quad (7)$$

and

$$\omega G_{ij}^{sd}(\omega) = \sum_{\ell} T_{i\ell}^{(s)} G_{\ell j}^{sd}(\omega) + \sum_{\ell} V_{sd}(R_i - R_{\ell}) G_{\ell j}^{dd}(\omega) + \langle S^Z \rangle_{\sigma} \sum_{\ell} J^{(s)}(R_i, R_{\ell}) G_{\ell j}^{sd}(\omega) \quad (8)$$

Equations (7) and (8) complete the determination of the $G_{ij}^{dd}(\omega)$ propagator within the adopted Hartree-Fock picture.

b) Zero order solution

In this paragraph we determine the host propagators, which will be used latter on in the first order correction. Since one has in this case translational symmetry: $\langle n_{i-\sigma}^{(d)} \rangle = \langle n_{-\sigma}^{(d)} \rangle = \langle n_d \rangle$ (last equality follows from the hypothesis of a paramagnetic host, and the absence of external fields).

Fourier transforming equations (5) - (8) and taking $J = 0$ one has:

$$(\omega - \epsilon_k^{(s)}) g_k^{ss}(\omega) = \frac{1}{2\pi} + V_{sd}(k) g_k^{ds}(\omega) \quad (9-a)$$

$$(\omega - E_k^{(d)}) g_k^{ds}(\omega) = V_{ds}(k) g_k^{ss}(\omega), \quad E_k^{(d)} = \epsilon_k^{(d)} + I \langle n_d \rangle \quad (9-b)$$

$$(\omega - E_k^{(d)}) g_k^{dd}(\omega) = \frac{1}{2\pi} + V_{ds}(k) g_k^{sd}(\omega) \quad (9-c)$$

$$(\omega - \epsilon_k^{(s)}) g_k^{sd}(\omega) = V_{sd}(k) g_k^{dd}(\omega) \quad (9-d)$$

In equations (9) we have used g instead of G to emphasize zero-order solutions.

Equations (9) can be solved to give:

$$g_k^{ss}(\omega) = \frac{1}{2\pi} \frac{\omega - E_k^{(d)}}{(\omega - \epsilon_k^{(s)})(\omega - E_k^{(d)}) - |V_{sd}(k)|^2} = \frac{1}{2\pi} \bar{g}_k^{ss}(\omega) \quad (10-a)$$

$$g_k^{dd}(\omega) = \frac{1}{2\pi} \frac{\omega - \epsilon_k^{(s)}}{(\omega - \epsilon_k^{(s)})(\omega - E_k^{(d)}) - |V_{sd}(k)|^2} = \frac{1}{2\pi} \bar{g}_k^{dd}(\omega) \quad (10-b)$$

$$g_k^{ds}(\omega) = \frac{V_{ds}(k)}{\omega - E_k^{(d)}} g_k^{ss}(\omega) \quad \text{and} \quad g_k^{sd}(\omega) = \frac{V_{sd}(k)}{\omega - \epsilon_k^{(s)}} g_k^{dd}(\omega) \quad (10-c)$$

From equations (10) one sees that given the band structure ($\epsilon_k^{(s)}$ and $E_k^{(d)}$) and the mixing matrix elements $|V_{sd}(k)|^2$ as a function of k the host propagators are completely specified (except for a numerical work of self-consistently determining $\langle n^d \rangle$ and the chemical potential μ).

c) First order perturbation solution

Now we solve, to first order in the exchange parameters, for the propagator $G_{ij}^{dd}(\omega)$; Fourier transforming equations (7) and (8) one gets:

$$\begin{aligned}
 (\omega - E_k^{(d)}) G_{kk'}^{(d)}(\omega) &= V_{ds}(k) G_{kk'}^{sd(1)}(\omega) + I \Delta n_{kk'}^{-\sigma(d)} \bar{g}_{k'}^{dd}(\omega) + \\
 &+ \langle S^Z \rangle \sigma J^{(d)}(k, k') \bar{g}_{k'}^{dd}(\omega)
 \end{aligned} \tag{11-a}$$

$$(\omega - \epsilon_k^{(s)}) G_{kk'}^{(s)}(\omega) = V_{sd}(k) G_{kk'}^{dd(1)}(\omega) + \langle S^Z \rangle \sigma J^{(s)}(k, k') \bar{g}_{k'}^{sd}(\omega) \tag{11-b}$$

Combining equations (11), and using the results (10) for host metal propagators one has (we defined $n_{kk'}^{-\sigma(d)} = \sum_i \Delta n_i^{-\sigma(d)} \frac{i(k-k')R_i}{e} = \Delta n_{k-k}^{-\sigma(d)}$):

$$\begin{aligned}
 \left\{ \omega - E_k^{(d)} - \frac{|V_{sd}(k)|^2}{\omega - \epsilon_k^{(s)}} \right\} G_{kk'}^{(d)}(\omega) &= \frac{1}{2\pi} \langle S^Z \rangle \sigma J^{(d)}(k, k') \bar{g}_{k'}^{dd}(\omega) + \\
 &+ \frac{1}{2\pi} I \Delta n_{kk'}^{-\sigma(d)} \bar{g}_{k'}^{dd}(\omega) + \frac{1}{2\pi} V_{ds}(k) \frac{1}{\omega - \epsilon_k^{(s)}} J^{(s)}(k, k') \langle S^Z \rangle \sigma \frac{1}{\omega - \epsilon_{k'}^{(s)}} V_{sd}(k') \bar{g}_{k'}^{dd}(\omega)
 \end{aligned} \tag{12}$$

Now if one changes $k \rightarrow k+q$ and $k' \rightarrow k$, the final result for the first order correction is:

$$\begin{aligned}
 G_{k+q, k}^{(d)}(\omega) &= \frac{1}{2\pi} \bar{g}_{k+q}^{dd}(\omega) J^{(d)}(k+q, k) \langle S^Z \rangle \sigma \bar{g}_k^{dd}(\omega) + \frac{1}{2\pi} \bar{g}_{k+q}^{dd}(\omega) I \Delta n_q^{-\sigma(d)} \bar{g}_k^{dd}(\omega) \\
 &+ \frac{1}{2\pi} \bar{g}_{k+q}^{dd}(\omega) V_{ds}(k+q) \frac{1}{\omega - \epsilon_{k+q}^{(s)}} J^{(s)}(k+q, k) \langle S^Z \rangle \sigma \frac{1}{\omega - \epsilon_k^{(s)}} V_{sd}(k) \bar{g}_k^{dd}(\omega)
 \end{aligned} \tag{13}$$

III) SOLUTION OF THE SELF-CONSISTENCY PROBLEM

a) Determination of the d-magnetization

Equation (13) shows clearly the scattering processes involved. The first term describes the scattering of wave vector k to $k+q$ induced by the exchange coupling of d electrons with the local moment. The second term describes the scattering by the fluctuation in occupation number of wave vector q , the source of coupling being the Coulomb interaction. Finally the last term describes how due to mixing effects, the d -electrons can feel the scattering produced by the coupling of s -states with the impurity. It should be emphasized that equation (13) involves a self-consistency problem through the existence of $\Delta n_q^{-\sigma}$, and now we proceed determining $\Delta n_q^{\sigma(d)}$ in terms of $\Delta n_q^{-\sigma(d)}$. One has:

$$\Delta n_q^{\sigma(d)} = \sum_k F_\omega |G_{k+q,k}^{dd(1)}(\omega)| \quad (14)$$

Introduce the following definitions:

$$\chi_{(o)}^{(d)}(k,q) = \frac{1}{2\pi} F_\omega \{ \bar{g}_{k+q}^{dd}(\omega) \bar{g}_k^{dd}(\omega) \} ; \chi_{(o)}^{(d)}(q) = \sum_k \chi_{(o)}^{(d)}(k,q) \quad (15-a)$$

$$\chi_{(o)}^{(d)}(k,q) = \frac{1}{2\pi} F_\omega \left\{ \bar{g}_{k+q}^{dd}(\omega) \frac{1}{\omega - \epsilon_{k+q}^{(s)}} \frac{1}{\omega - \epsilon_k^{(s)}} \bar{g}_k^{dd}(\omega) \right\} = \quad (15-b)$$

$$= \frac{1}{2\pi} F_\omega \left\{ \bar{g}_{k+q}^{ss}(\omega) \frac{1}{\omega - E_{k+q}^{(d)}} \frac{1}{\omega - E_k^{(d)}} \bar{g}_k^{ss}(\omega) \right\}$$

$$\chi^{(s)}(k,q) = \frac{1}{2\pi} F_{\omega} \{ \bar{g}_{k+q}^{ss}(\omega) \bar{g}_k^{ss}(\omega) \} \quad (15-c)$$

The explicit form of the "susceptibilities" will be given later on (cf. appendix 1) in terms of the band structure and mixing matrix elements. Using definitions (14) and (15) one gets from (13)

$$\Delta n_q^{\sigma(d)} = I \chi_{(o)}^{(d)}(q) \Delta n_q^{-\sigma(d)} + \langle S^z \rangle \sigma \{ \sum_k J^{(d)}(k+q,k) \chi_{(o)}^{(d)}(k,q) \} + \quad (16-a)$$

$$+ \sum_k J^{(s)}(k+q,k) V_{ds}(k+q) V_{sd}(k) \chi_{(o)}(k,q) = I \chi_{(o)}^{(d)}(q) \Delta n_q^{-\sigma(d)} + \langle S^z \rangle \sigma M(q)$$

Changing spin indices one has:

$$\Delta n_q^{-\sigma(d)} = I \chi_{(o)}^{(d)}(q) \Delta n_q^{\sigma(d)} - \langle S^z \rangle \sigma M(q) \quad (16-b)$$

Combining equations (16) one has:

$$\Delta n_q^{\sigma(d)} = \sigma \langle S^z \rangle \frac{M(q)}{1 + I \chi_{(o)}^{(d)}(q)} \quad (17)$$

One should note that $\chi_{(o)}^{(d)}(q)$ differs from the usual one by a minus sign (cf. Appendix). From (17) one gets for the induced d-magnetization.

$$m_q^{(d)} = 2 \frac{\langle S^Z \rangle}{1 + I \chi_{(o)}^{(d)}(q)} \sum_k \left\{ J^{(d)}(k+q, k) \chi_{(o)}^{(d)}(k, q) + J^{(s)}(k+q, k) V_{ds}(k+q) V_{sd}(k) \chi_{(o)}^{(d)}(k, q) \right\} \quad (18)$$

Expression (18) can be used to introduce effective exchange coupling; one rewrites (18) as:

$$m_q^{(d)} = 2 \langle S^Z \rangle \sum_k J_{\text{eff}}^{(d)}(k+q, k) \left\{ 1 + \frac{J^{(s)}(k+q, k)}{J^{(d)}(k+q, k)} V_{ds}(k+q) V_{sd}(k) \frac{\chi_{(o)}^{(d)}(k, q)}{\chi_{(o)}^{(d)}(k, q)} \right\} \frac{\chi_{(o)}^{(d)}(k, q)}{1 + I \chi_{(o)}^{(d)}(q)} \quad (19)$$

Equation (19) suggests the following definition

$$J_{\text{eff}}^{(d)}(k+q, k) = J^{(d)}(k+q, k) \left\{ 1 + \frac{J^{(s)}(k+q, k)}{J^{(d)}(k+q, k)} V_{ds}(k+q) V_{sd}(k) \frac{\chi_{(o)}^{(d)}(k, q)}{\chi_{(o)}^{(d)}(k, q)} \right\} \quad (20)$$

Using the exchange enhanced susceptibility

$$\chi_{(o)}^{(d)}(k, q) = \frac{\chi_{(o)}^{(d)}(k, q)}{1 + I \chi_{(o)}^{(d)}(q)}$$

one finally gets for the induced d-magnetization:

$$\bar{m}_q^{(d)} = 2 \langle S^Z \rangle \sum_k J_{\text{eff}}^{(d)}(k+q, k) \chi^{(d)}(k, q) \quad (21)$$

This result is the natural generalization of the usual result

$$\bar{m}_q^{(d)} = 2 \langle S^Z \rangle \sum_k J^{(d)}(k+q, k) \chi^{(d)}(k, q)$$

occurring for a d band in absence of mixing effects.

b) Determination of the s-magnetization

Now it remains to determine the s-magnetization; the first order contribution of equation (5) and (6), in Fourier representation is:

$$(\omega - \epsilon_k^{(s)}) G_{kk'}^{ss(i)}(\omega) = V_{sd}(k) G_{kk'}^{ds(i)}(\omega) + \langle S^Z \rangle J^{(s)}(k, k') g_{k'}^{ss}(\omega) \quad (22-a)$$

$$(\omega - \epsilon_k^{(d)}) G_{kk'}^{ds(i)}(\omega) = V_{ds}(k) G_{kk'}^{ss(i)}(\omega) + \{ J^{(d)}(k, k') \langle S^Z \rangle + I \Delta n_{kk'}^{(d)} \} g_{k'}^{ds}(\omega) \quad (22-b)$$

Combining equations (22) and using equation (10) one gets:

$$\begin{aligned} G_{k+q, k}^{ss(i)}(\omega) &= \frac{1}{2\pi} \bar{g}_{k+q}^{ss}(\omega) J^{(s)}(k+q, k) \langle S^Z \rangle \bar{g}_k^{ss}(\omega) + \\ &+ \frac{1}{2\pi} \bar{g}_{k+q}^{ss}(\omega) V_{sd}(k+q) \frac{1}{\omega - \epsilon_{k+q}^{(d)}} \{ J^{(d)}(k+q, k) \langle S^Z \rangle + I \Delta n_q^{(d)} \} \frac{1}{\omega - \epsilon_k^{(d)}} V_{ds}(k) \bar{g}_k^{ss}(\omega) \end{aligned} \quad (23)$$

One gets then:

$$m_q^{(s)} = 2 \langle S^Z \rangle \sum_k \{ J^{(s)}(k+q, k) \chi^{(s)}(k, q) + \bar{J}^{(d)}(k+q, k) V_{ds}(k) \chi_{(o)}^{(s)}(k, q) \} \quad (27)$$

Expression (27) suggests finally the definition of an effective exchange:

$$J_{\text{eff}}^{(s)}(k+q, k) = J^{(s)}(k+q, k) \left\{ 1 + \frac{\bar{J}^{(d)}(k+q, k)}{J^{(s)}(k+q, k)} V_{sd}(k+q) V_{ds}(k) \frac{\chi_{(o)}^{(s)}(k, q)}{\chi^{(s)}(k, q)} \right\} \quad (28)$$

Which show a great formal similarity with its d-counter part, equation (20); the induced s-magnetization is then:

$$m_q^{(s)} = 2 \langle S^Z \rangle \sum_k J_{\text{eff}}^{(s)}(k+q, k) \chi^{(s)}(k, q) \quad (29)$$

Combining equations (29) and (21) one gets for the total induced magnetization:

$$m_q = 2 \langle S^Z \rangle \sum_k \{ J_{\text{eff}}^{(s)}(k+q, k) \chi^{(s)}(k, q) + J_{\text{eff}}^{(d)}(k+q, k) \chi^{(d)}(k, q) \} \quad (30)$$

When s-d mixing is absent expression (30) becomes

$$m_q^{(o)} = 2 \langle S^Z \rangle \sum_k \{ J^{(s)}(k+q) \chi^{(s)}(k, q) + J^{(d)}(k+q, k) \chi^{(d)}(k, q) \}$$

where $J^{(s)}$ and $J^{(d)}$ are the "bare" exchange couplings.

IV) DISCUSSIONS AND CONCLUSIONS

We have shown that the induced magnetization for the s-d coupled bands is still given by the sum of the s and d contributions, provided that effective exchange couplings are introduced (cf. equation (30)). The s and d susceptibilities are the mainly s and d contributions to the susceptibility and its explicit form, ready for numerical computation is presented in Appendix I. It is interesting to compare the relative importance of the corrections arising from the mixing to the "bare" exchange couplings $J^{(s)}(k+q,k)$ and $J^{(d)}(k+q,k)$. Comparing equations (20) and (28) one sees that the correction to the d exchange is of the order of $(J^{(s)}/J^{(d)}) (\chi_{(o)}/\chi_d)$ and that of the s exchange is of the order of $(J^{(d)}/J^{(s)}) (\chi_{(o)}/\chi_s)$. Since one usually has $\chi_d \gg \chi_s$ and $J^{(d)} > J^{(s)}$ for rare earths one expects a bigger correction for $J_{\text{eff}}^{(s)}$ than for $J_{\text{eff}}^{(d)}$. This is the result already obtained [5], using a phenomenological description for the effects of s-d mixing. In that paper [5] it was concluded that $J_{\text{eff}}^{(s)}$ could even change of sign if the ratio $\chi^{(d)}/\chi^{(s)}$ is large enough. Expressions (20) and (28) suggest that numerical studies should be made in order to obtain, in terms of the band structure, the behaviour of the effective exchange couplings as a function of q.

APPENDIX I

In this appendix we give explicit expressions for the involved susceptibilities; from (15-a) one has:

$$\chi_{(o)}^{(d)}(k,q) = \frac{1}{2\pi} F_{\omega} \left\{ \frac{\omega - \epsilon_{k+q}^{(s)}}{(\omega - E_{k+q}^{(1)})(\omega - E_{k+q}^{(2)})} \times \frac{\omega - \epsilon_k^{(s)}}{(\omega - E_k^{(1)})(\omega - E_k^{(2)})} \right\} \quad (\text{A-1})$$

where the energies $E_k^{(1)}$ and $E_k^{(2)}$ are the solutions of the equation:

$$(\omega - \epsilon_k^{(s)}) (\omega - E_k^{(d)}) - |V_{sd}(k)|^2 = 0 \quad (\text{A-2})$$

Rewriting (A-1) in terms of partial fractions one gets:

$$\chi_{(o)}^{(d)}(k, q) = \sum_{\mu, \nu=1}^2 (-1)^{\mu+\nu} F_{\omega} \left\{ \frac{(\omega - \epsilon_{k+q}^{(s)}) (\omega - \epsilon_k^{(s)})}{(E_{k+q}^{(1)} - E_{k+q}^{(2)}) (E_k^{(1)} - E_k^{(2)}) (E_{k+q}^{(\mu)} - E_k^{(\nu)})} \frac{1}{2\pi} \left[\frac{1}{\omega - E_{k+q}^{(\mu)}} - \frac{1}{\omega - E_k^{(\nu)}} \right] \right\} \quad (\text{A-3})$$

Explicit calculation of the F_{ω} symbol gives the final result:

$$\chi_{(o)}^{(d)}(k, q) = \sum_{\mu, \nu=1}^2 (-1)^{\mu+\nu} \frac{(E_{k+q}^{(u)} - \epsilon_{k+q}^{(s)}) (E_{k+q}^{(u)} - \epsilon_k^{(s)}) f(E_{k+q}^{(u)}) - (E_k^{(v)} - \epsilon_{k+q}^{(s)}) (E_k^{(v)} - \epsilon_k^{(s)}) f(E_k^{(v)})}{(E_{k+q}^{(1)} - E_{k+q}^{(2)}) (E_k^{(1)} - E_k^{(2)}) (E_{k+q}^{(u)} - E_k^{(v)})} \quad (\text{A-4})$$

A quite similar expression can be obtained for $\chi_{(o)}^{(s)}(k, q)$ just replacing where it appears s by d , in expression (A-4).

Finally, proceeding in a similar way one gets for $\chi_{(o)}(k, q)$

$$\chi_{(o)}(k, q) = \sum_{\mu, \nu=1}^2 (-1)^{\mu+\nu} \frac{f(E_{k+q}^{(\mu)}) - f(E_k^{(\nu)})}{(E_{k+q}^{(1)} - E_{k+q}^{(2)}) (E_k^{(1)} - E_k^{(2)}) (E_{k+q}^{(\mu)} - E_k^{(\nu)})} \quad (\text{A-5})$$

Expression (A-4) and (A-5) together with (A-2) connect the susceptibilities to the band structure. In the above expressions one frequently encounters $f(\epsilon_k) - f(\epsilon_{k+q})$ in order to ensure positive values for the susceptibility.

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