

Functional Integral Approach to Itinerant two Sublattice Magnetic Systems: Degeneracy Effects

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We have studied the magnetization as a function of temperature for two sublattice itinerant electron systems, using the functional integral formalism and taking into account the degeneracy of the d band. A numerical application is made to a model transition metal intermetallic.

I. Introduction

In a recent paper^[1] we have applied the functional integral approach, in the static approximation, to describe the finite temperature magnetic properties of the transition metal Laves phase intermetallics. In order to simplify the formulation and to make easier the numerical calculations for these intermetallics, composed by two sublattices, some approximations had to be introduced.

The first approximation is to adopt a single band Hubbard like Hamiltonian, considering five identical "d" subbands. The second approximation concerns to the description of the two sublattices of the intermetallic. The homothetic band approach was used; in this approach one starts from the dispersion relation associated with the B sublattice, to which a model density of state is associated. The corresponding dispersion relation for the A sublattice is proportional to the B one

and includes in general an energy shift.

The comparison between the numerical results obtained in that work^[1] and the experimental data for the transition temperature, indicated that this picture should be improved. In this work we extend our previous calculation^[1] to take into account the degeneracy of the d band, but keeping all the other approximations. The inclusion of the degeneracy of the "d" band enables to account for the exchange effects on the magnetization and transition temperature of the intermetallic. The introduction of this term in the Hamiltonian makes the calculation very complicated, but we hope to get a higher magnetic transition temperature, as compared to^[1].

II. Hamiltonian

We start with the Hamiltonian including the degeneracy of the d band and adapted to describe two sublattice systems:

$$H = H_0 + H_1^A + H_1^B, \quad (1)$$

$$\begin{aligned}
 H_0 = & \sum_{lr\sigma} \epsilon_{0r}^A a_{lr\sigma}^+ a_{lr\sigma} + \sum_{ll'rr'\sigma} T_{ll'rr'}^{AA} a_{lr\sigma}^+ a_{l'r'\sigma} + \epsilon_{0r}^B a_{jr\sigma}^+ a_{jr\sigma} + \\
 & + \sum_{jj'rr'\sigma} T_{jj'rr'}^{BB} a_{jr\sigma}^+ a_{j'r'\sigma} + \sum_{ljrr'\sigma} T_{ljrr'}^{AB} (a_{lr\sigma}^+ a_{j'r'\sigma} + a_{j'r'\sigma}^+ a_{lr\sigma}), \quad (2)
 \end{aligned}$$

$$H_1^A = \frac{1}{2} U^A \sum_{lr\sigma} n_{lr\sigma}^A n_{lr-\sigma}^A + \frac{1}{9} \bar{U}^A \sum_{l\sigma r \neq r'} n_{lr\sigma}^A n_{l'r-\sigma}^A + \frac{1}{2} (\bar{U}^A - J^A) \sum_{l\sigma r \neq r'} n_{lr\sigma}^A n_{l'r'\sigma}^A, \quad (3)$$

$$H_1^B = \frac{1}{2} U^B \sum_{jr\sigma} n_{jr\sigma}^B n_{jr-\sigma}^B + \frac{1}{2} \bar{U}^B \sum_{j\sigma r \neq r'} n_{jr\sigma}^B n_{j'r-\sigma}^B + \frac{1}{2} (\bar{U}^B - J^B) \sum_{j\sigma r \neq r'} n_{jr\sigma}^B n_{j'r'\sigma}^B, \quad (4)$$

where $a_{lr\sigma}^+$ ($a_{jr\sigma}$) is the creation (annihilation) operator of one electron with spin σ at the l (j) site in the r sub band ($r = 1...5$). ϵ_{0r}^A (ϵ_{0r}^B) is the d energy center of the r -subband associated to the A (B) sublattice. The terms $T_{ll'rr'}^{AA}$ ($T_{jj'rr'}^{BB}$) represent the electron hopping between ll' (jj') sites of the same A (B) sublattice and $T_{ljrr'}^{AB}$ is the hopping between sites of different sublattice. U^A (U^B) is the local Coulomb energy interaction associated with the d electrons in the same subband of the A (B) sublattice; \bar{U}^A (\bar{U}^B) is the local Coulomb energy interaction associated with the d electrons in the different subbands of the A (B) sublattice. Finally J^A (J^B) is the local exchange energy interaction of the “ d ” electrons in different subbands associated to the same sublattice. It was shown in the literature^[2] that the interaction terms of the above Hamiltonian (H_1^A, H_1^B) may be put in the following form

$$I = -\frac{1}{4} \sum_{lr r'} (n_{lr}^A C_{rr'}^A n_{l'r'}^A + m_{lr}^A \bar{C}_{rr'}^A m_{l'r'}^A) \quad (5.a)$$

$$H_1^B = -\frac{1}{4} \sum_{jr r'} (n_{jr}^B C_{rr'}^B n_{j'r'}^B + m_{jr}^B \bar{C}_{rr'}^B m_{j'r'}^B) \quad (5.b)$$

where $n_{lr}^A = \sum_{\sigma} a_{lr\sigma}^+ a_{lr\sigma}$; $m_{lr}^A = \sum_{\sigma} \sigma n_{lr\sigma}$ with similar quantities for the B sublattice and C^I and \bar{C}^I ($I = A$ or B) are matrices which elements are given by:

$$C_{rr'}^I = -(2\bar{U}^I - J^I) - (U^I - 2\bar{U}^I + J^I) \delta_{rr'} \quad (6.a)$$

$$\bar{C}_{rr'}^I = J^I + (U^I - J^I) \delta_{rr'} \quad (6.b)$$

III. The Partition Function

In order to calculate the partition function of the system described by the above Hamiltonian, we follow the standard procedure used in the literature^[3], namely Feynman’s time ordering operator T_0 . In this way, this partition function may be written as:

$$\begin{aligned}
 Z = & T_0 T_0 e^{-\int_0^\beta H_0 ds} e^{-\int_0^\beta ds \frac{1}{4} \sum_{lr r'} (n_{lr}^A C_{rr'}^A n_{l'r'}^A + m_{lr}^A \bar{C}_{rr'}^A m_{l'r'}^A)} \times \\
 & \times e^{-\int_0^\beta ds \frac{1}{4} \sum_{jr r'} (n_{jr}^B C_{rr'}^B n_{j'r'}^B + m_{jr}^B \bar{C}_{rr'}^B m_{j'r'}^B)}, \quad (7)
 \end{aligned}$$

where β is given by $1/k_B T$.

Using the generalized Hubbard-Stratonovici relation^[4]:

$$e^{\pm \sum_{ij} t_{ij} D_{ij} t_{ij}} = N^{-1} \int dx e^{-\sum_{ij} x_{ij} (D_{ij}^{-1}) x_{ij} - \sum_l \sqrt{\mp 1} t_l x_l}, \quad (8.a)$$

where N is given by:

$$N = \int dx e^{-\sum_{ij} x_j (D_{ji}^{-1}) x_i - \sum_j \sqrt{\Xi} \Gamma_i x_j}, \quad (8.b)$$

We can write the above partition function as:

$$\begin{aligned} Z = & Tr T_0 e^{-\int_0^\beta ds H_0} \int \prod_{lr} dx_{lr}^A dy_{lr}^A \left(e^{-\int_0^\beta ds \sum_{lrr'} x_{lr}^A (C_{rr'}^A)^{-1} x_{lr'}^A - i x_{lr}^A n_{lr}^A} \right. \\ & \left. e^{-\int_0^\beta ds \sum_{lrr'} y_{lr}^A (\bar{C}_{rr'}^A)^{-1} y_{lr'}^A - y_{lr}^A m_{lr}^A} \right) \times \\ & \times \int \prod_{jr} dx_{jr}^B dy_{jr}^B \left(e^{-\int_0^\beta ds \sum_{jrr'} x_{jr}^B (C_{rr'}^B)^{-1} x_{jr'}^B - i x_{jr}^B n_{jr}^B} \right. \\ & \left. e^{-\int_0^\beta ds \sum_{jrr'} y_{jr}^B (\bar{C}_{rr'}^B)^{-1} y_{jr'}^B - y_{jr}^B m_{jr}^B} \right), \quad (9) \end{aligned}$$

where x_{lr}^A and y_{lr}^A are charge and spin fluctuating fields at the sites l of the A sublattice and associated to the r subband. Similar notation holds for the B sublattice. From here on we disregard the factor N , since it appears in numerator and denominator of the averaged values. This partition function involves implicitly an integration over the time dependence s of the fluctuating fields. At this point we introduce our first simplification, namely the static approximation, that neglects the time dependence. So one has:

$$Z = \int \prod_{lr} dx_{lr}^A dy_{lr}^A \int \prod_{jr} dx_{jr}^B dy_{jr}^B e^{-\beta(\Psi(x_{lr}^A, y_{lr}^A, x_{jr}^B, y_{jr}^B))} \quad (10)$$

where

$$\Psi(x_{lr}^A, y_{lr}^A, x_{jr}^B, y_{jr}^B) = \Psi_0(x_{lr}^A, y_{lr}^A, x_{jr}^B, y_{jr}^B) + \Psi_1(x_{lr}^A, y_{lr}^A, x_{jr}^B, y_{jr}^B), \quad (11.a)$$

$$\begin{aligned} \Psi_0(x_{lr}^A, y_{lr}^A, x_{jr}^B, y_{jr}^B) = & \sum_{lrr'} (x_{lr}^A (C_{rr'}^A)^{-1} x_{lr'}^A + y_{lr}^A (\bar{C}_{rr'}^A)^{-1} y_{lr'}^A) + \\ & \sum_{jrr'} (x_{jr}^B (C_{rr'}^B)^{-1} x_{jr'}^B + y_{jr}^B (\bar{C}_{rr'}^B)^{-1} y_{jr'}^B), \quad (11.b) \end{aligned}$$

$$\Psi_1(x_{lr}^A, y_{lr}^A, x_{jr}^B, y_{jr}^B) = -\frac{1}{\beta} \ln Tr e^{-\beta \tilde{H}_0(x_{lr}^A, y_{lr}^A, x_{jr}^B, y_{jr}^B)}, \quad (11.c)$$

$$\tilde{H}_0 = H_0 - \sum_{lr} (i x_{lr}^A n_{lr}^A + y_{lr}^A m_{lr}^A) - \sum_{jr} (i x_{jr}^B n_{jr}^B + y_{jr}^B m_{jr}^B). \quad (11.d)$$

In expression (10), in spite of the use of the static approximation, the calculation of this partition function is still very complex, due to a multiple integration over the charge and the spin fields associated to each sublattice. We can simplify this calculation defining a suitable set of new variables, reflecting the symmetry of the lattice. Suppose here that each sublattice of our model intermetallic has cubic symmetry. Then, we use the well known irreducible representations, (t_{2g} and e_g), to transform the old charge and spin fields (x, y) into new

field variables (v, χ). The result is:

$$v_{lr}^I = \sum_{r'} R_{rr'} x_{lr'}^I, \quad \chi_{lr}^I = \sum_{r'} R_{rr'} y_{lr'}^I \quad (12.a)$$

or the inverse transform:

$$x_{lr}^I = \sum_{r'} (R_{rr'}^{-1}) v_{lr'}^I, \quad y_{lr}^I = \sum_{r'} (R_{rr'}^{-1}) \chi_{lr'}^I \quad (12.b)$$

where the R transformation matrix for this symmetry^[2] is given by

$$\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 2 & -1 & -1 & 0 & 0 \\ 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & -1 \end{bmatrix}. \quad (13)$$

Using this transformation, we can write Ψ_0 and Ψ_1 in terms of the new variables in a simpler way. Firstly,

the term Ψ_0 may be rewritten as:

$$\begin{aligned} \Psi_0 = & \sum_{lrr'} (\nu_{lr}^A D_{rr'}^A \nu_{lr'}^A + \xi_{lr}^A \bar{D}_{rr'}^A \xi_{lr}^A) + \\ & + \sum_{jrr'} (\nu_{jr}^B D_{rr'}^B \nu_{jr'}^B + \xi_{jr}^B \bar{D}_{rr'}^B \xi_{jr}^B), \end{aligned} \quad (14)$$

where D^I and \bar{D}^I are matrices given by

$$D_{rr'}^I = (R_{rr'}^{-1})^T (C_{rr'}^I)^{-1} R_{rr'}^{-1}, \quad \bar{D}_{rr'}^I = (R_{rr'}^{-1})^T (C_{rr'}^I)^{-1} R_{rr'}^{-1}, \quad (15)$$

with seven non-vanishing elements for each sublattice

$$D_{11}^I = \frac{(U^I + 2\bar{U}^I - J^I)}{3(U^I + 8\bar{U}^I - 4J^I)(2\bar{U}^I - U^I - J^I)}, \quad (16.a)$$

$$D_{33}^I = D_{55}^I = 3D_{22}^I = \frac{(U^I + 8\bar{U}^I - 4J^I)}{2(U^I + 8\bar{U}^I - 4J^I)(2\bar{U}^I - U^I - J^I)}, \quad (16.b)$$

$$D_{44}^I = \frac{(U^I + 4\bar{U}^I - 4J^I)}{2(U^I + 8\bar{U}^I - 4J^I)(2\bar{U}^I - U^I - J^I)}, \quad (16.c)$$

$$D_{14}^I = D_{41}^I = \frac{(J^I - 2\bar{U}^I)}{(U^I + 8\bar{U}^I - 4J^I)(2\bar{U}^I - U^I - J^I)}, \quad (16.d)$$

$$\bar{D}_{11}^I = \frac{(U^I + J^I)}{3(U^I + 4J^I)(U^I - J^I)}, \quad (17.a)$$

$$\bar{D}_{33}^I = \bar{D}_{55}^I = 3\bar{D}_{22}^I = \frac{(U^I + 4J^I)}{2(U^I + 4J^I)(U^I - J^I)}, \quad (17.b)$$

$$\bar{D}_{44}^I = \frac{(U^I + 2J^I)}{2(U^I + 4J^I)(U^I - J^I)}, \quad (17.c)$$

$$D_{14}^I = D_{41}^I = \frac{-J^I}{(U^I + 4J^I)(U^I - J^I)}, \quad (17.d)$$

and zero otherwise.

At this point we use the saddle point approximation to eliminate some charge and spin fields^[2]; we obtain for each sublattice:

$$\nu_2^I = \nu_3^I = \nu_5^I = 0, \quad \xi_2^I = \xi_3^I = \xi_5^I = 0. \quad (18)$$

In this way the only non vanishing elements of (14) are those involving D_{11}^I , D_{44}^I , D_{14}^I , D_{41}^I , and similarly for the terms involving \bar{D}^I . Remembering the dimensions of the irreducible representations for the cubic symmetry group, we define the following fluctuating fields^[2]

$$\begin{aligned} \nu_{j1}^I &= 3\nu_{jt}^I; & \xi_{j1}^I &= 3\xi_{jt}^I \\ \nu_{j4}^I &= 2\nu_{je}^I; & \xi_{j4}^I &= 3\xi_{je}^I \end{aligned} \quad (19)$$

where t and e represent t_{2g} and e_g subbands respectively. With these transformations, equation (14) finally takes the form

$$\Psi_0 = \Psi_0^A + \Psi_0^B \quad , \quad (20.a)$$

$$\Psi_0^A = \sum_t 9D_{tt}^A \nu_{it}^2 + 4D_{ee}^A \nu_{ie}^2 + 12D_{te}^A \nu_{it}^A \nu_{ie}^A + 9\bar{D}_{tt}^A \xi_{it}^2 + 4\bar{D}_{ee}^A \xi_{ie}^2 + 12\bar{D}_{te}^A \xi_{it}^A \xi_{ie}^A \quad , \quad (20.b)$$

$$\Psi_0^B = \sum_j 9D_{tt}^B \nu_{jt}^2 + 4D_{ee}^B \nu_{je}^2 + 12D_{te}^B \nu_{jt}^B \nu_{je}^B + 9\bar{D}_{tt}^B \xi_{jt}^2 + 4\bar{D}_{ee}^B \xi_{je}^2 + 12\bar{D}_{te}^B \xi_{jt}^B \xi_{je}^B \quad , \quad (20.c)$$

where

$$\begin{aligned} D_{tt}^I &= D_{11}^I & \bar{D}_{tt}^I &= \bar{D}_{11}^I \\ D_{ee}^I &= D_{44}^I & \bar{D}_{ee}^I &= \bar{D}_{44}^I \\ D_{te}^I &= D_{14}^I = D_{41}^I & \bar{D}_{te}^I &= \bar{D}_{14}^I = \bar{D}_{41}^I \end{aligned} \quad (21)$$

It remains now to transform equation (11.c) using the same procedure; in this particular case, this corresponds to rewrite the Hamiltonian (11.d) using the transformation (12.b). One gets

$$\tilde{H}_0 = H_0 - \sum_{lr} (i\nu_{lr}^A + \sigma \xi_{lr}^A) w_{lr}^A - \sum_{jr} (i\nu_{jr}^B + \sigma \xi_{jr}^B) w_{jr}^B \quad , \quad (22)$$

where w_{jr}^I is a column vector defined by $(R^{-1})^T n_{jr}^I$, with elements given by

$$\begin{bmatrix} w_{j1}^I \\ w_{j2}^I \\ w_{j3}^I \\ w_{j4}^I \\ w_{j5}^I \end{bmatrix} = \begin{bmatrix} (n_{j1}^I + n_{j2}^I + n_{j3}^I)/3 \\ (2n_{j1}^I - n_{j2}^I - n_{j3}^I)/6 \\ (n_{j2}^I - n_{j3}^I)/2 \\ (n_{j4}^I + n_{j5}^I)/2 \\ (n_{j4}^I - n_{j5}^I)/2 \end{bmatrix} \quad (23)$$

Let us note that, the occupation number of each subband, cubic symmetry, is equal to

$$\begin{aligned} \langle n_{j1}^I \rangle &= \langle n_{j2}^I \rangle = \langle n_{j3}^I \rangle = \langle n_{jt}^I \rangle \\ \langle n_{j4}^I \rangle &= \langle n_{j5}^I \rangle = \langle n_{je}^I \rangle \quad . \end{aligned} \quad (24)$$

In this situation, the only non zero elements in (23) are $w_{j1}^I w_{j4}^I$; this fact together with (18), resulting from the saddle point approximation to the charge and spin fields, implies that we can rewrite this Hamiltonian \tilde{H}_0 (22) in the same form of the Hamiltonian (2), replacing the energy levels ϵ_{0r}^I by the following effective spin dependent energies

$$\epsilon_{lr\sigma}^I = \epsilon_0^I - (i\nu_{lr}^I + \sigma \xi_{lr}^I) \quad , \quad (25.a)$$

where now $r = t$ or e , representing the t_{2g} and e_g subband. The Hamiltonian becomes then:

$$\begin{aligned} \tilde{H}^0 &= \sum_{lr\sigma} \epsilon_{lr\sigma}^A a_{lr\sigma}^+ a_{lr\sigma} + \sum_{ll'r\sigma} T_{ll'r\sigma}^{AA} a_{lr\sigma}^+ a_{l'r\sigma} \\ &+ \sum_{jr\sigma} \epsilon_{jr\sigma}^B a_{jr\sigma}^+ a_{jr\sigma} + \sum_{jj'r\sigma} T_{jj'r\sigma}^{BB} a_{jr\sigma}^+ a_{j'r\sigma} \\ &+ \sum_{ljr\sigma} T_{ljr\sigma}^{AB} (a_{lr\sigma}^+ a_{jr\sigma} + a_{jr\sigma}^+ a_{lr\sigma}) \quad . \end{aligned} \quad (25.b)$$

IV. Self consistent equations

This new Hamiltonian \tilde{H}_0 can be considered as describing an alloy, with an intrinsic disorder associated to the fluctuating fields; these obey a distribution probability given by

$$P(\xi_t^A \xi_e^A \nu_t^A \nu_e^A \xi_t^B \xi_e^B \nu_t^B \nu_e^B) = \frac{e^{-\beta \Psi(\xi_t^A \xi_e^A \nu_t^A \nu_e^A \xi_t^B \xi_e^B \nu_t^B \nu_e^B)}}{\int d\xi_t^A d\xi_e^A d\nu_t^A d\nu_e^A d\xi_t^B d\xi_e^B d\nu_t^B d\nu_e^B e^{-\beta \Psi(\xi_t^A \xi_e^A \nu_t^A \nu_e^A \xi_t^B \xi_e^B \nu_t^B \nu_e^B)}} \quad . \quad (26)$$

In order to treat this disordered Hamiltonian we can use the CPA approximation^[3]; introducing the effective media $\sum_{r\sigma}^A (\sum_{r\sigma}^B)$ to restore translation invariance, we obtain the effective Hamiltonian (H^{eff}):

$$H^{eff} = \tilde{H}^0(\Sigma_{r\sigma}^A \Sigma_{r\sigma}^B) + H^A + H^B, \quad (27.a)$$

where the above unperturbed Hamiltonian $\tilde{H}^0(\Sigma_{r\sigma}^A \Sigma_{r\sigma}^A)$ has the same form of (25.b) with the self energy ($\Sigma_{r\sigma}^I$) replacing the spin dependent energy levels ($\epsilon_{lr\sigma}^I$). The term H^A (H^B) is the local perturbation at l_0 and j_0 sites of the A (B) sublattice, given by

$$H^A = \sum_{\sigma r} (\epsilon_{lr\sigma}^A - \Sigma_{r\sigma}^A) a_{l_0 r \sigma}^+ a_{l_0 r \sigma} = \sum_{\sigma r} V_{r\sigma}^A a_{l_0 r \sigma}^+ a_{l_0 r \sigma} \quad (27.8)$$

$$H^B = \sum_{\sigma r} (\epsilon_{jr\sigma}^B - \Sigma_{r\sigma}^B) a_{j_0 r \sigma}^+ a_{j_0 r \sigma} = \sum_{\sigma r} V_{r\sigma}^B a_{j_0 r \sigma}^+ a_{j_0 r \sigma} \quad (27.c)$$

Using the irreducible representation of the cubic symmetry, the Green's function of the two coupled sublattice system, defined by the effective Hamiltonian (27.a), may be represented by the following matrix, with spin implicitly included

$$\begin{bmatrix} G_{tt}^{AA} & 0 & G_{tt}^{AB} & 0 \\ 0 & G_{ee}^{AA} & 0 & G_{ee}^{AB} \\ G_{tt}^{BA} & 0 & G_{tt}^{BB} & 0 \\ 0 & G_{ee}^{BA} & 0 & G_{ee}^{BB} \end{bmatrix}. \quad (28)$$

This propagator should satisfy the matrix Dyson's equation

$$G = g + gVG, \quad (29)$$

where the unperturbed Green's functions (g), associated with Hamiltonian $\tilde{H}^0(\Sigma_{r\sigma}^A \Sigma_{r\sigma}^A)$, defined in terms of the self energy, has a similar form as (28) and the matrix potential (V) is given by the 2×2 matrix

$$\begin{bmatrix} V_t^A & 0 & 0 & 0 \\ 0 & V_e^A & 0 & 0 \\ 0 & 0 & V_t^B & 0 \\ 0 & 0 & 0 & V_e^B \end{bmatrix}. \quad (30)$$

Following the same procedure of [1] to solve Dyson's equation, we obtain the propagator for the $I = A, B$ sublattice as

$$G_{ll'r}^{II} = \bar{g}_{ll'r}^{II} + \bar{g}_{ll_0 r}^{II} \frac{V_r^I}{(1 - V_r^I \bar{F}_r^I)} \bar{g}_{l_0 l'r}^{II}, \quad (31)$$

where renormalized propagator \bar{g}^{II} above is defined as in [1] by

$$\bar{g}_{ll'r}^{AA} = g_{ll'r}^{AA} + g_{lj_0 r}^{AB} \frac{V_r^B}{(1 - V_r^B \bar{F}_r^B)} g_{j_0 l'r}^{BA}, \quad (32.a)$$

$$\bar{g}_{jj'r}^{BB} = g_{jj'r}^{BB} + g_{jl_0 r}^{BA} \frac{V_r^A}{(1 - V_r^A \bar{F}_r^A)} g_{l_0 j'r}^{AB}. \quad (32.b)$$

The propagator (32.a) renormalizes the motion of electrons in the r subband, between sites of the same A sublattice, including a hopping at j_0 site to the B sublattice, where they are scattered by the local potential V_r^B and a hopping back to the A sublattice; a similar interpretation holds for (32.b). In equation (31), the renormalized local Green's function \bar{F}^A and \bar{F}^B are defined from (32) as $\bar{g}_{ll'r}^{AA}$ and $\bar{g}_{jj'r}^{BB}$ respectively; similarly F^A and F^B are defined as $g_{jj'r}^{AA}$ and $g_{jj'r}^{BB}$. The unperturbed Green's functions (g), involving the two sublattices, are calculated using the homothetic band approach^[1]. In this approximation, we start from given dispersion relations ϵ_{kr} ($r = t, e$) for the B sublattice and assume the dispersion relations for the A sublattice to be proportional to ϵ_{kr} with a coefficient α_r . The coupling between sublattices again is proportional to ϵ_{kr} , with coefficient γ_r . So the unperturbed Green's function has the form

$$g(k, z) = \begin{bmatrix} z - \Sigma_{t\sigma}^A - \alpha_t \epsilon_{kt} & 0 & -\gamma_t \epsilon_{kt} & 0 \\ 0 & z - \Sigma_{e\sigma}^A - \alpha_e \epsilon_{ke} & 0 & -\gamma_e \epsilon_{ke} \\ -\gamma_t \epsilon_{kt} & 0 & z - \Sigma_{t\sigma}^B - \epsilon_{kt} & 0 \\ 0 & \gamma_e \epsilon_{ke} & 0 & z - \Sigma_{e\sigma}^B - \epsilon_{ke} \end{bmatrix}^{-1} \quad (33)$$

The unperturbed Green's function (intra and inter sublattice) associated with the r subband are explicitly given by:

$$F_{r\sigma}^A(z) = g_{lr\sigma}^{AA}(z) = \frac{1}{(\alpha_r - \gamma_r^2)(E_{r\sigma}^+ - E_{r\sigma}^-)} [(z - \Sigma_{r\sigma}^B - E_{r\sigma}^-)F(E_{r\sigma}^-) - (z - \Sigma_{r\sigma}^B - E_{r\sigma}^+)F(E_{r\sigma}^+)] , \quad (34.a)$$

$$F_{r\sigma}^B(z) = g_{jr}^{BB}(z) = \frac{1}{(\alpha_r - \gamma_r^2)(E_{r\sigma}^+ - E_{r\sigma}^-)} [(z - \Sigma_{r\sigma}^A - \alpha E_{r\sigma}^-)F(E_{r\sigma}^-) - (z - \Sigma_{r\sigma}^A - \alpha E_{r\sigma}^+)F(E_{r\sigma}^+)] , \quad (34.b)$$

$$g_{ij\sigma}^{AB}(z) = \frac{\gamma_r}{Z_N(\alpha_r - \gamma_r^2)(E_{r\sigma}^+ - E_{r\sigma}^-)} [E_{r\sigma}^- (E_{r\sigma}^- F(E_{r\sigma}^-) - 1 - E_{r\sigma}^+) (E_{r\sigma}^+ F(E_{r\sigma}^+) - 1)] , \quad (34.c)$$

$$E_{r\sigma}^\pm = \frac{1}{2(\alpha_r - \gamma_r^2)} \{ [(z - \Sigma_{r\sigma}^A + \alpha(z - \Sigma_{r\sigma}^B))] \pm \{ [z - \Sigma_{r\sigma}^A + \alpha(z - \Sigma_{r\sigma}^B)]^2 - 4[(z - \Sigma_{r\sigma}^A)(z - \Sigma_{r\sigma}^B)](\alpha_r - \gamma_r^2) \}^{1/2} \} , \quad (34.d)$$

where Z_N is the number of nearest neighbours and $F_r(E_{r\sigma}^\pm)$ is the Hilbert transform of the density of states $\rho_r(\epsilon)$, given by

$$F_r(E_{r\sigma}^\pm) = \int d\epsilon \frac{\rho_r(\epsilon)}{(E_{r\sigma}^\pm - \epsilon)} . \quad (35)$$

Taking the average of (31), remembering that $\langle G_{jjr}^{AA} \rangle = \bar{g}_{jjr}^{AA}$ and the $\langle G_{ijr}^{BB} \rangle = \bar{g}_{ijr}^{BB}$, the effective media $\Sigma_{r\sigma}^A$ and $\Sigma_{r\sigma}^B$ may be obtained from the following equations

$$\int d\xi_t^A d\xi_e^A d\nu_t^A d\nu_e^A d\xi_t^B d\xi_e^B d\nu_t^B d\nu_e^B \frac{P(\xi_t^A \xi_e^A \nu_t^A \nu_e^A \xi_t^B \xi_e^B \nu_t^B \nu_e^B) V_{r\sigma}^A(\xi_r^A \nu_r^A)}{1 - V_{r\sigma}^A(\xi_r^A \nu_r^A) \bar{F}_{r\sigma}^A(\xi_t^A \xi_e^A \nu_t^A \nu_e^A \xi_t^B \xi_e^B \nu_t^B \nu_e^B)} = 0 , \quad (36.a)$$

$$\int d\xi_t^A d\xi_e^A d\nu_t^A d\nu_e^A d\xi_t^B d\xi_e^B d\nu_t^B d\nu_e^B \frac{P(\xi_t^A \xi_e^A \nu_t^A \nu_e^A \xi_t^B \xi_e^B \nu_t^B \nu_e^B) V_{r\sigma}^B(\xi_r^B \nu_r^B)}{1 - V_{r\sigma}^B(\xi_r^B \nu_r^B) \bar{F}_{r\sigma}^B(\xi_t^A \xi_e^A \nu_t^A \nu_e^A \xi_t^B \xi_e^B \nu_t^B \nu_e^B)} = 0 , \quad (36.b)$$

where $P(\xi_t^A \xi_e^A \nu_t^A \nu_e^A \xi_t^B \xi_e^B \nu_t^B \nu_e^B)$ is the probability distribution defined by relation (26) where the free energy Ψ is explicitly given by[2]

$$\begin{aligned} \Psi(\xi_t^A \xi_e^A \nu_t^A \nu_e^A \xi_t^B \xi_e^B \nu_t^B \nu_e^B) &= \Psi_0(\xi_t^A \xi_e^A \nu_t^A \nu_e^A \xi_t^B \xi_e^B \nu_t^B \nu_e^B) + \\ &+ \frac{3}{\pi} \int dz f(z) \text{Im} \sum_{\sigma} \ln[1 - V_{t\sigma}^A(\xi_t^A \nu_t^A) \bar{F}_{t\sigma}^A(z)] + \\ &+ \frac{2}{\pi} \int dz f(z) \text{Im} \sum_{\sigma} \ln[1 - V_{e\sigma}^A(\xi_e^A \nu_e^A) \bar{F}_{e\sigma}^A(z)] \\ &+ \frac{3}{\pi} \int dz f(z) \text{Im} \sum_{\sigma} \ln[1 - V_{t\sigma}^B(\xi_t^B \nu_t^B) \bar{F}_{t\sigma}^B(z)] + \\ &+ \frac{2}{\pi} \int dz f(z) \text{Im} \sum_{\sigma} \ln[1 - V_{e\sigma}^B(\xi_e^B \nu_e^B) \bar{F}_{e\sigma}^B(z)] , \end{aligned} \quad (37)$$

where $f(z)$ is the Fermi distribution function and $z = \epsilon + i\delta$, $\delta \rightarrow 0+$. The expressions (36) form a coupled set of two self consistent equations, for each r symmetry. These involve difficult multiple integrations over the fluctuating fields of both sublattices, and must be solved simultaneously.

In order to simplify the numerical calculations, we neglect the the second order terms (g^{AB} . g^{BA}). In this way, the renormalized local Green's functions $\bar{F}^B(\bar{F}^A)$ defined through (32), reduce in this approximation to $F^B(F^A)$ and the probability distribution may be written as

$$P(\xi_t^A \xi_e^A \nu_t^A \nu_e^A \xi_t^B \xi_e^B \nu_t^B \nu_e^B) = P^A(\xi_t^A \xi_e^A \nu_t^A \nu_e^A) \cdot P^B(\xi_t^B \xi_e^B \nu_t^B \nu_e^B); \quad (38.a)$$

where

$$P^I(\xi_t^I \xi_e^I \nu_t^I \nu_e^I) = \frac{e^{-\beta \Psi^I(\xi_t^I \xi_e^I \nu_t^I \nu_e^I)}}{\int d\xi_t^I d\xi_e^I d\nu_t^I d\nu_e^I e^{-\beta \Psi^I(\xi_t^I \xi_e^I \nu_t^I \nu_e^I)}} \quad I = A \text{ or } B \quad (38.b)$$

With

$$\begin{aligned} \Psi^I(\xi_t^I \xi_e^I \nu_t^I \nu_e^I) &= \Psi_0^I(\xi_t^I \xi_e^I \nu_t^I \nu_e^I) + \frac{3}{\pi} \int dz f(z) \text{Im} \sum_{\sigma} \ln[1 - V_{t\sigma}^I(\xi_t^I \nu_t^I) F_{t\sigma}^I(z)] \\ &+ \frac{2}{\pi} \int dz d(z) \text{Im} \sum_{\sigma} \ln[1 - V_{\sigma}^I \xi_e^I \nu_e^I F_{\sigma}^I(z)]. \end{aligned} \quad (38.c)$$

Note that due to this simplification, one ends up with two independent free energies, each one associated to the corresponding sublattice. A subtle point is that the inter sublattice coupling is incorporated implicitly via the functions $F_{r\sigma}^I$.

Using this approximation, the self consistent equations that determine the effective media reduce to

$$\int d\xi_t^A d\xi_e^A d\nu_t^A d\nu_e^A \frac{V_{r\sigma}^A(\xi_r^A \nu_r^A)}{1 - V_{r\sigma}^A(\xi_r^A \nu_r^A) F_{r\sigma}^A(z)} P^A(\xi_t^A \xi_e^A \nu_t^A \nu_e^A) = 0, \quad (39.a)$$

$$\int d\xi_t^B d\xi_e^B d\nu_t^B d\nu_e^B \frac{V_{r\sigma}^B(\xi_r^B \nu_r^B)}{1 - V_{r\sigma}^B(\xi_r^B \nu_r^B) F_{r\sigma}^B(z)} P^B(\xi_t^B \xi_e^B \nu_t^B \nu_e^B) = 0. \quad (39.b)$$

Now, for each r symmetry we have two self consistent equations, indirectly coupled via the Green's function $F_{r\sigma}^I$. These equations involve an integration over charge and spin fields. As it is often made in the literature^[3] we can eliminate the integrations over the charge field, by using the saddle point approximation, where the charge fields are replaced by

$$\begin{bmatrix} -i\nu_t^I \\ -i\nu_e^I \end{bmatrix} = \begin{bmatrix} (U + 4\bar{U}^I - 2J^I)/2 & (2\bar{U}^I - J^I) \\ 3 & 2 - 2 \end{bmatrix} \begin{bmatrix} n_t^I \\ n_e^I \end{bmatrix}, \quad (40)$$

and the occupation number at $r = t, e$ subbands of the I sublattice is

$$n_r^I = \sum_{\sigma} n_{r\sigma}^I = -\frac{1}{\pi} \int d\epsilon f(\epsilon) \text{Im} \sum_{\sigma} F_{r\sigma}^I(z); \quad z = \epsilon + i\delta, \quad \delta \rightarrow 0^+, \quad (41)$$

the Green's function $F_{r\sigma}^I(z)$ being given by (34).

The magnetic moment associated to the r subband of each sublattice, is calculated using the standard procedure of the functional integral method^[3]:

$$m_t^I = 6\bar{D}_{tt} \langle \xi_t^I \rangle + 4\bar{D}_{te} \langle \xi_e^I \rangle, \quad (42.a)$$

$$m_e^I = 6\bar{D}_{te} \langle \xi_t^I \rangle + 4\bar{D}_{ee} \langle \xi_e^I \rangle, \quad (42.b)$$

the mean value being given by:

$$\langle \xi_r^I \rangle = \frac{\int d\xi_t^I d\xi_e^I \xi_r^I e^{-\beta \Psi^I(\xi_t^I \xi_e^I)}}{\int d\xi_t^I d\xi_e^I e^{-\beta \Psi^I(\xi_t^I \xi_e^I)}}. \quad (42.c)$$

The magnetic moment for each sublattice is

$$M^I = 3m_t^I + 2m_e^I. \quad (42.S)$$

V. Numerical results

In this section we illustrate the formalism developed here applying it to the case of $ZrFe_2$ Laves phase intermetallic, with two sublattices $A = Zr$ and $B = Fe$. If the degeneracy in the Laves phase case is to be described rigorously, we need three irreducible representations; for the sake of simplicity we assume in this

illustration the existence of only two irreducible representations t_{2g} and e_g . In this first approach we take identical densities of states associated to the different irreducible representations.

Note that other characteristics of the Laves phase lattice are included in our picture, via the inter-sublattice hopping, explicitly considered in the formalism. In what concerns one electron states, the present calculation is identical to that reported in [1]. We conclude that here, the important effect of the degeneracy is to introduce the Coulomb and exchange interactions between different orbitals, not considered in the non-degenerate version [1].

We start assuming the model density of states adopted in a previous work [5], extracted from Terao and Shimizu's tight binding calculation [6]. This model density of states enables the numerical solution of the coupled equations (39), for a given set of parameters which we specify now.

Firstly we adopt the following occupation numbers, for A and B sublattice, and for each subband as: $n_t^B = n_e^B = 1.457$ and $n_t^A = n_e^A = 0.505$. Also, a series of parameters should have their values estimated; these parameters are the Coulomb and exchange interaction strengths. We adopted, to illustrate our results, the following values: $U^A = 0.3$, $\bar{U}^A = 0.1$, $J^A = 0.05$, $U^B = 0.6$, $\bar{U}^B = 0.3$, $J^B = 0.1$, all these being in units of half-band width. We recall that 3d wave functions of Fe are more contracted than the 4d ones associated to Zr. We expect then higher values for the Coulomb interactions in the 3d case as shown above.

Another series of parameters already introduced in [1] are the α and γ values, parametrizing respectively the homothetic 3d, 4d bands and the inter sublattice hopping. It has been shown by Yamada and Shimizu [7], that the hybridization between the spin polarized 3d states and the higher energy states associated to the 4d or 5d atoms, plays a central role in explaining the occurrence of ferromagnetism in these compounds. In the previous calculation [5] it is shown that allowing to a spin dependence of the γ parameter, the stability of a ferrimagnetic phase is ensured at $T = 0K$. This is done by properly adjusting the γ values. The numerical values of the above parameters, independent of the

subband, are taken equal to those adopted in [1], where these values were obtained for low temperatures. The remaining parameters were adjusted in such a way that the low temperature saturation magnetization fits to the observed data.

The parameter space is a quite rich one and the specific role of each parameter requires a special study; in this work we only want to illustrate the effect of the exchange interactions in producing changes in the Curie temperature. Here we show the following new result: including degeneracy, only via the Coulomb and Exchange interactions, a change by a factor of the order 3 in the value of the transition temperature is obtained, as compared to [1].

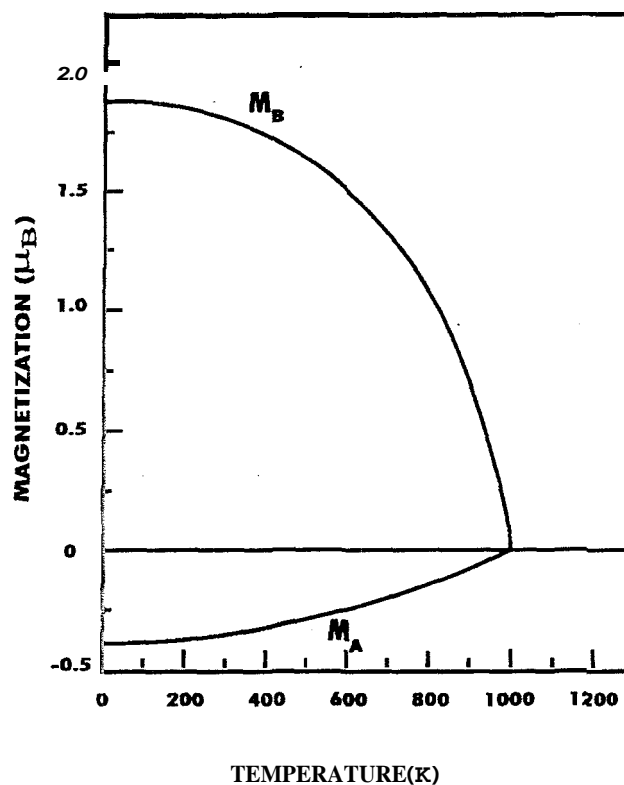


Figure 1. Temperature dependence of the magnetization (in units of μ_B) for A and B sublattice.

In figure 1 is presented the temperature dependence of the magnetization in units of μ_B for both sublattices. Let us emphasize that a closer agreement with the experimental value of T_c requires the explicit introduction of more detailed one electron densities of states, compatible with Laves phase symmetry.

In conclusion, even in the case of more complex systems like Laves phase compounds with stable rare

earths, discussed within a combined Monte Carlo functional integral method^[8], the present formalism can improve the agreement with the experiments, in what concerns the transition temperature.

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