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Chemical and structural disorder effects on the Curie temperature

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Abstract

The disorder effects on the Curie temperature of ferromagnetic and ferroelectric systems are studied by factorizing the spin-spin (or dipole-dipole) interaction in a chemical (on-site) and structural (off-site) part. Assuming the statistical independence of the two contributions, the Curie temperature T_c is calculated in the limit of small disorder and in the mean field approximation. The chemical disorder always enhances T_c . In the absence of spin waves (Ising-like systems), the structural disorder enhances T_c in turn. The only negative contribution to T_c is found in Heisenberg-like systems, and is ascribed to the interplay between structural disorder and spin waves. A comparison is made with other mean-field theories, that adopt a different representation of the disorder. The application of the results obtained to real systems is considered, with special reference to recent experimental data on ferroelectric perovskites. An approximated expression, consistent with the mean field approach, is suggested to estimate the relative weight of the chemical and structural disorder effects, even when an exact factorization is impossible, as it is the case of the *exchange* interactions.

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1 Introduction

The modifications induced by disorder on ferromagnetic and ferroelectric systems is a long standing question [1, 2] that continues to stimulate a very

active field of investigations, both theoretical and experimental. From the experimental viewpoint [3, 4, 5, 6], the reported data seem to escape from any attempt to classify the disorder effects in a general and simple scheme. The increase or decrease of the Curie temperature T_c , for instance, is still an open question. Data referring to pure mechanical treatments (for example, milling), tend to favor the decrease of T_c with increasing disorder [6]. This agrees, qualitatively, with earliest theoretical results [7]. In random alloys, most of the measured data are concerned with the non monotonic behavior of T_c , as a function of the *average* concentration of various magnetic or non magnetic components [8]. The disorder, resulting from the random *fluctuations* about those average values, is especially studied in connection to the changes of the magnetization [3, 4], while the effects on T_c itself are usually neglected. For ferroelectrics, recent experimental data and theoretical models [5, 9, 10] report about the increase of T_c with increasing cationic disorder.

The earliest theories predict no disorder effects on the T_c of Ising-like systems [11], and a depression of T_c in Heisenberg-like systems [7]. More recently, contrasting theoretical results have been reported for ferromagnetic Anderson-Hubbard models, some pointing to an increase of T_c [12, 13], others pointing to a decrease [14]. In the present work we study the simplest possible case of a *direct* interaction between localized spins, i.e. a lattice $\{r\}$ of sites, each occupied by a spin s_r , with interaction energy $U(r, r') s_r s_{r'}$. More elaborated dynamical models, involving the indirect coupling through itinerant electrons [15, 16] and the Mott-Hubbard interaction [12, 13, 14], are ignored in what follows. Though we speak about "spins" for brevity, it is intended that the present approach can be extended to electric dipoles too.

The basic elements entering the spin interactions can be split into two main classes: *chemical* and *structural*. The formers account for the on-site features (atomic orbitals, local electric dipoles or magnetic moments, etc.), while the latter account for the off-site features, typically the spin-spin relative positions. In order to study their distinct disorder effects, we assume a model interaction in which the chemical and structural features are factorized:

$$U(r, r') = -\lambda_r \lambda_{r'} J(r - r') . \quad (1)$$

The on site-parameters λ_r 's, with probability distribution P_λ , are statistically independent from the random positions $\{r\}$'s of the lattice sites. Hence, the off-site couplings $J(r - r')$'s are themselves random variables, with a probability distribution P_J , independent from P_λ . We call "average crystal", with Curie temperature $T_{(J, \lambda)}$, the ordered system with interaction energy $\langle \lambda_r \lambda_{r'} \rangle \langle J(r - r') \rangle$, where $\langle \dots \rangle$ indicates the average over P_λ

and/or P_J . In contrast, $\langle\langle \dots \rangle\rangle$ will indicate a mean value including the thermal average too. Though $T_{\langle J, \lambda \rangle}$ does not refer, in general, to any real crystal, it represents a convenient reference value, with respect to which one studies the enhancement or depression of T_c with increasing chemical-structural fluctuations. In view of studying the disorder effects to the lowest significant order, we shall refer to the so called disordered crystal model, i.e. a lattice $\{r\}$ whose sites $r = f + u_f$ are slightly shifted with respect to a reference crystalline lattice $\{f\}$, by a random displacement u_f ($|u_f| \ll$ first nearest neighbor distance). Taking advantage of the one-to-one correspondence between $\{r\}$ and $\{f\}$, all the quantities can be expressed in terms of the reference crystal lattice. In particular, the coupling $J(r - r')$ reads, on setting $\rho_{ff'} = u_f - u_{f'}$:

$$J(r - r') = J_{ff'} = J(f - f') + \frac{\partial J(f - f')}{\partial f_\alpha} \rho_{ff'}^\alpha + \frac{1}{2} \frac{\partial^2 J(f - f')}{\partial f_\alpha \partial f_{\alpha'}} \rho_{ff'}^\alpha \rho_{ff'}^{\alpha'} + \dots, \quad (2)$$

to second order in the displacements, where α numerates the spatial cartesian components and the summation over repeated indices is intended. In this case, the structural disorder is described by the probability distribution $P_\rho(\rho)$ of the random anti-symmetric variable $\rho_{f'f} = -\rho_{ff'}$. In Sections 2 and 3 it will be shown that the random fluctuations always *enhance* the Curie temperature, with the exception of the structural disorder in **Heisenberg**-like systems (see Table 1 for a qualitative summary). In this case the overall effect on T_c turns out to be model-dependent. This is due to the existence of a negative contribution [7], that is argued to reflect the interplay between structural disorder and spin waves.

T_c	Chemical	Structural
Ising	+	+
Heisenberg	+	\pm model-dependent

Table 1: Effects of disorder (chemical and structural) on T_c of Ising and Heisenberg-like systems. + and - indicate enhancement and depression respectively

In Section 4, the present results will be compared with those obtained in refs [7, 11], in which the interaction energy $U(r, r')$ is assumed as an overall random variable, without distinction between structural and chemical disorder.

In Section 5, the applications of the model interaction eq.n (1) to real systems are discussed. The model fits well with ferroelectric systems, since λ_r , carrying the chemical disorder, can be related to the magnitude of the on-site dipole, and the coupling function $J(r - r')$ is influenced only by the structural disorder, through the relative position $r - r'$. Experimental evidences supporting the results of Section 2 have been actually reported, in the context of ferroelectrics perovskites [5, 9]. An alternative theory, specific for ferroelectrics, has been already formulated [10], with results quite consistent with those obtained in Section 2.

The application of eq.n (1) to ferromagnets with *exchange* interactions is less immediate, due to the impossibility of an exact separation of chemical and structural components, when those are nested in an exchange integral. However, an approximate method is proposed for estimating the relative weight of chemical and structural disorder in this case too.

It should be clear that eq.n (2) can be applied also to the thermal atomic displacements in an otherwise perfect crystal. The resulting modification of T_c will be calculated in Section 5.

2 Disorder effects on Ising-like systems

For Ising-like model we mean an array of \mathcal{N} semi-classical spins s_g , all oriented along the z-axis, and ranging over a set Λ of discrete or continuous values (for simplicity, we assume the same Λ for all the spins). In this static approximation, the set of magnetic energies E depends on a \mathcal{N} -component vector $\mathbf{s} = s_{g_1}, s_{g_2} \dots, s_{g_{\mathcal{N}}}$. From eq.n (1) one has:

$$E(\mathbf{s}) = -\frac{1}{2} \sum'_{g,f} \lambda_g \lambda_f s_g s_f J_{gf}, \quad (3)$$

where the prime in the sum means $g \neq f$. For ferromagnetic systems, one can assume $J > 0$ and $\lambda_g > 0$. According to the MF approximation, the energy E in eq.n (3) is replaced by a sum $E_{mf} = (1/2) \sum_g \epsilon_g$ of single-site energies [17, 18]:

$$\epsilon_g(s_g | \hat{\mathbf{s}}) = -s_g \lambda_g \sum_{f \neq g} \lambda_f \hat{s}_f J_{gf}, \quad (4)$$

in which \hat{s}_f is the thermal mean value of the spin variable s_f . The self consistent equation, determining \hat{s}_g then reads:

$$\hat{s}_g = \frac{\sum_{s \in \Lambda} e^{-\beta \epsilon_g(s | \hat{\mathbf{s}})} s}{\sum_{s \in \Lambda} e^{-\beta \epsilon_g(s | \hat{\mathbf{s}})}} = F \left(\beta \lambda_g \sum_{f \neq g} \lambda_f \hat{s}_f J_{gf} \right). \quad (5)$$

If Λ (the array of the spin values) is symmetric with respect to zero, i.e., each value of the spin is present with both signs, the function F in eq.n (5) has the following properties [19]:

$$F^{(2n)}(0) = 0 \text{ for each } n \ ; \ \dot{F}(0) > 0 \ ; \ \ddot{F}(0) < 0. \quad (6)$$

One main point in eq.n (1), is the possibility of rescaling the s_r 's and defining new interacting variables $S_r = \lambda_r s_r$. While studying the S_r 's or the s_r 's is perfectly equivalent, in an exact calculation, this is not the case in a MF approach in which either $\langle\langle S_r \rangle\rangle$ or $\langle\langle s_r \rangle\rangle$ are assumed site-independent. In both cases, the approximation involved is neglecting the statistical correlations between the interacting variables. In the latter case, however, one neglects also the correlations between the s_r 's and the λ_r 's. In fact, passing to the dressed spins S_g , equation (5) reads:

$$\hat{S}_g = \lambda_g F \left(\beta \lambda_g \sum_{f \neq g} \hat{S}_f J_{gf} \right) = \Phi_g \left(\lambda_g, \hat{\mathbf{S}} \right). \quad (7)$$

Equation (7) contains the on-site disorder only through the parameter λ_g . Therefore \hat{S}_g is statistically independent from the other λ 's, while \hat{s}_g is not (eq.n (5)). This shows that the correct procedure is calculating $\langle\langle S \rangle\rangle$, then, possibly, expressing $\langle\langle s \rangle\rangle$ as $\langle\lambda^{-1}\rangle\langle\langle S \rangle\rangle$.

The quantity of interest is the joint probability distribution $P_{joint}(\hat{\mathbf{S}})$ of the dressed spin values. Neglecting the correlations of the \hat{S}_g 's means assuming $P_{joint}(\hat{\mathbf{S}}) = \prod_g P_S(\hat{S}_g)$. Setting $x_g = \beta \hat{S}_g$, the equation for the probability distribution $P(x_g)$ becomes, from eq.n (7):

$$P(x_g) = \int dP_\lambda \prod_{f \neq g} dx_f P(x_f) dP_\rho(\rho_{gf}) \delta(\beta \Phi_g - x_g), \quad (8a)$$

where

$$\Phi_g(\lambda, \mathbf{x}) = \lambda F \left(\lambda \sum_{f \neq g} x_f J_{gf} \right), \quad (8b)$$

and $dP_\lambda = P_\lambda d\lambda$, $dP_\rho = P_\rho d\rho$ account for on-site and off-site disorder respectively (recall eq.n (2)). The mean value $\langle\langle S \rangle\rangle = \kappa T \langle x \rangle$ and the standard deviation $\sigma_S = \kappa T \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$ of the dressed spins follow from the two coupled equations:

$$\langle x \rangle = \int dx P(x) x = \beta \langle \lambda F \rangle \ ; \ \langle x^2 \rangle = \int dx P(x) x^2 = \beta^2 \langle \lambda^2 F^2 \rangle, \quad (9)$$

according to eq.n.s (8). On setting:

$$\langle \rho \rangle = 0, \lambda = 1 + \Delta\lambda, x = \langle x \rangle + \Delta x \quad (10a)$$

$$\langle \Delta\lambda \rangle = \langle \Delta x \rangle = 0 \quad (10b)$$

$$\langle \rho_\alpha^2 \rangle = \sigma_\rho^2, \langle \Delta\lambda^2 \rangle = \sigma_\lambda^2, \langle \Delta x^2 \rangle = \sigma_x^2, \quad (10c)$$

one defines the fluctuations of the random variables about their mean values and the corresponding square standard deviations. The first relation (10a) means that the reference crystal and the average crystal coincide. The second relation (10a) means that $\langle \lambda \rangle = 1$, which can be assumed without loss of generality (possibly on rescaling J). The first relation (10c) refers to each of the cartesian components of ρ , that we assume to be independent from one another and identically distributed. The system of equations (9) is obtained by expanding the integrand in (8a) to the lowest significant order in the fluctuations Δx , $\Delta\lambda$ and ρ . This results in the following expressions:

$$\begin{aligned} \frac{\langle x \rangle}{\beta} &= F(\theta) + \dot{F}(\theta) \langle x \rangle (\sigma_\lambda^2 J_0 + \sigma_\rho^2 J_2) + \\ &+ \frac{\ddot{F}(\theta)}{2} [\langle x \rangle^2 \sigma_\lambda^2 J_0^2 + \langle x \rangle^2 \sigma_\rho^2 w_1^2 + \sigma_x^2 J_1^2], \end{aligned} \quad (11a)$$

$$\begin{aligned} \frac{\langle x^2 \rangle}{\beta^2} &= (1 + \sigma_\lambda^2) F^2(\theta) + \\ &+ 2F(\theta) \langle x \rangle \left[\sigma_\rho^2 J_2 F(\theta) \dot{F}(\theta) + 2\sigma_\lambda^2 \ddot{F}(\theta) J_0 \right] + \\ &+ \left[\dot{F}^2(\theta) + \ddot{F}(\theta) F(\theta) \right] [\langle x \rangle^2 \sigma_\lambda^2 J_0^2 + \langle x \rangle^2 \sigma_\rho^2 w_1^2 + \sigma_x^2 J_1^2] \end{aligned} \quad (11b)$$

in which (recall eq.n (2)):

$$J_0 = \sum_{D \neq 0} J(D), \quad J_1^2 = \sum_{D \neq 0} J^2(D) \quad (12a)$$

$$J_2 = \frac{1}{2} \sum_{D \neq 0} \nabla_D^2 J, \quad J_3^2 = \sum_{D \neq 0} (\nabla_D J)^2 \quad (12b)$$

are site-independent parameters, due to the sum over the reference crystal sites, and

$$\theta = \langle x \rangle J_0. \quad (12c)$$

In order to calculate the Curie temperature T_c , one looks for the solutions of the equation system (11) by an appropriate expansion of the functions F , \dot{F} and \ddot{F} in θ or $\langle x \rangle$ (eq.n (12c)), up to $\langle x \rangle^3$. Recalling eq.ns (6), one gets, for the non trivial solutions ($\langle x \rangle \neq 0$):

$$\langle x \rangle^2 = \frac{\kappa T_{\langle \rho, \lambda \rangle}}{A} \left[1 + \sigma_\lambda^2 + \sigma_\rho^2 J_2 - \sigma_x^2 \frac{J_1^2 |\ddot{F}(0)|}{2\dot{F}(0)} - \frac{T}{T_{\langle \rho, \lambda \rangle}} \right] \geq 0 \quad (13a)$$

and

$$\sigma_x^2 = \langle x^2 \rangle - \langle x \rangle^2 = \langle x \rangle^2 \frac{4 [\sigma_\lambda^2 + \sigma_\rho^2 J_2 / J_0] + \sigma_\rho^2 J_3^2 / J_0^2}{(T/T_{\langle \rho, \lambda \rangle})^2 - J_1^2 / J_0^2} \geq 0, \quad (13b)$$

in which

$$\kappa T_{\langle \rho, \lambda \rangle} = \dot{F}(0) J_0 \quad (14a)$$

defines the Curie temperature of the reference (or average) crystal, and

$$A = \frac{|\ddot{F}(0)|}{6} J_0^3 (1 + 6\sigma_\lambda^2 + 3\sigma_\rho^2 J_3^2 / J_0^2) \quad (14b)$$

is a positive constant. On substituting eq.n (13b) in eq.n (13a), it is immediately seen that $\langle x \rangle \propto \sqrt{1 - T/T_c}$ for $T < T_c$, where

$$T_c = T_{\langle \rho, \lambda \rangle} (1 + \sigma_\lambda^2 + \sigma_\rho^2 J_2) \quad (15)$$

is the Curie temperature including the disordered effects to lowest order. It is seen that T_c increases with increasing chemical disorder. If J_2 (eq.n (12a)) is positive, which is the standard case, for $J(D)$ positive and decreasing with $|D|$, the structural disorder does enhance T_c in turn. It is intended that equations (13) apply for T close to T_c , which is, in turn, close to $T_{\langle \rho, \lambda \rangle}$. This ensures that σ_x^2 (eq.n (13b)) is positive. In fact J_0^2/J_1^2 (eq.ns (12a)) is certainly larger than 1, since it represents an effective number of first nearest neighbors (the exact number, actually, if J is a constant, coupling only the first nearest neighbors).

If one were to follow the same procedure adopted above, to calculate $\langle\langle s \rangle\rangle$ according to eq.n (5), it is not difficult to see that the result would be simply $T_c = T_{\langle \rho, \lambda \rangle} (1 + \sigma_\rho^2 J_2)$, i.e. the absence of any *chemical* disorder effect on the Curie temperature. In fact, in eq.n (5) the random variables λ 's refer to different sites, so that all the bilinear terms $\Delta\lambda_g\Delta\lambda_f$ vanish in

average. In contrast, Φ_g in eq.n (7) depends only on λ_g . This yields the term

$$\beta \dot{F}(\theta) \langle x \rangle \sigma_\lambda^2 J_0 \quad (16)$$

(eq.n (11a)), that is responsible for the relative increment σ_λ^2 of the Curie temperature in eq.n(15). As mentioned above, assuming $\langle \langle s_g \rangle \rangle$ site-independent introduces an additional error with respect to the same assumptions on $\langle \langle S_g \rangle \rangle$. Setting $x_g = \beta \hat{s}_g$, an estimate of this error is given by the correlation term

$$\begin{aligned} c_{hg} &= \langle \lambda_h x_g \rangle - \langle \lambda_h \rangle \langle x_g \rangle = \\ &= -\beta \int \prod_{f'} dP_\lambda(\lambda_{f'}) \Delta \lambda_h \prod_{f \neq g} dP(x_f) dP_\rho(\rho_{gf}) \times \\ &\quad \times F \left(\lambda_g \sum_{f \neq g} \lambda_f x_f J_{gf} \right) \end{aligned}$$

(recall eq.n (5)). On expanding F to first order in the $\Delta \lambda_{g,f}$'s and in the ρ_{gf} 's, the preceding equation yields

$$c_{hg} = \beta \sigma_\lambda^2 \langle x \rangle J(g-h) \dot{F}(\langle x \rangle J_0) .$$

Recalling the definition (12c), the sum

$$\sum_h c_{hg} = \beta \langle x \rangle \sigma_\lambda^2 J_0 \dot{F}(\theta) \quad (17)$$

gives the total error, that coincides exactly with the term eq.n (16). Hence, the absence of chemical disorder effects in the Curie temperature $T_c = T_{\langle \rho, \lambda \rangle} (1 + \sigma_\rho^2 J_2)$, calculated under the assumption $\langle \langle s_f \rangle \rangle$ site-independent, results from neglecting the statistical correlations between the λ_h 's and the \hat{s}_g 's. This error is exactly compensated by the increase of the Curie temperature, calculated for the dressed spins $S_g = \lambda_g s_g$.

3 Disorder effects on Heisenberg-like systems

The simplest example of Heisenberg ferromagnet is an array of Pauli spins \vec{s}_i , interacting through the coupling energy eq.n (1). This leads to the following Hamiltonian:

$$H = -\frac{1}{2} \sum'_{l,h} J_{lh} \lambda_l \lambda_h \vec{s}_l \vec{s}_h = \quad (18a)$$

$$= \frac{1}{2} \sum'_{l,h} J_{lh} \lambda_l \lambda_h \left[n_l - b_l^\dagger b_h - n_l n_h \right], \quad (18b)$$

in which, passing from (18a) to (18b), the spin components

$$s_g^x = b_g + b_g^\dagger, \quad s_g^y = i(b_g^\dagger - b_g), \quad s_g^z = (1 - 2b_g^\dagger b_g) \quad (19)$$

have been expressed in terms of the creation-annihilation operators b_g^\dagger , b_g . Those obey Bosonic and Fermionic commutation rules for $f \neq g$ and $f = g$, respectively [20]. In particular:

$$[b_f, b_g^\dagger] = \delta_{fg} (1 - 2n_g), \quad n_f = b_f b_f^\dagger. \quad (20)$$

Following the same procedure as in Section 2, we define the dressed spins $\vec{S}_f = \lambda_f \vec{s}_f$ and the corresponding operators $B_f^\dagger = \lambda_f b_f^\dagger$, $B_f = \lambda_f b_f$ such that, from (20):

$$[B_f, B_g^\dagger] = \delta_{fg} (\lambda_f^2 - 2N_f), \quad S_f^z = \left(\lambda_f - 2\frac{N_f}{\lambda_f} \right), \quad N_f = B_f B_f^\dagger. \quad (21)$$

The Hamiltonian (18a) then becomes:

$$H = 2 \sum'_{l,h} J_{lh} \left[\frac{\lambda_l}{\lambda_h} N_l - B_l^\dagger B_h - \frac{N_l N_h}{\lambda_l \lambda_h} \right]. \quad (22)$$

Following the seminal work of Zubarev [21] and the development by Montgomery *et al* [7], one defines the time dependent two-site Green function $G_{gf}(t-t') = \langle B_g(t); B_f^\dagger(t') \rangle_T$, which motion equation:

$$i \frac{dG_{gf}(t-t')}{dt} = \delta(t-t') \langle [B_g(t), B_f^\dagger(t)] \rangle_T + \langle [B_g(t), H]; B_f^\dagger(t') \rangle_T. \quad (23)$$

Note that in the present section the thermal average is indicated as $\langle \dots \rangle_T$, instead of $\langle \dots \rangle$. On time-Fourier transforming

$$G_{gf}(t-t') = \int_{-\infty}^{\infty} d\omega e^{-i\omega(t-t')} \widehat{G}_{gf}(\omega),$$

equation (23) can be put in the matricial form:

$$\delta_{gf} = 2\pi \sum_l \left[\left\{ \frac{\omega}{\lambda_g S} - 2 \sum_h J_{hg} \right\} \delta_{lg} + 2J_{lg} \right] \widehat{G}_{lf}(\omega) \quad (24)$$

under the following approximations:

$$\langle N_l(t) B_g(t); B_f^\dagger(t') \rangle_T = \langle N_l(t) \rangle_T \langle B_g(t); B_f^\dagger(t') \rangle_T \quad (25a)$$

$$\lambda_g - 2\langle N_g \rangle_T / \lambda_g = \langle S_g^z \rangle_T = S \quad \text{independent from } g. \quad (25b)$$

Equation (25a) corresponds to decoupling the hierarchy of the higher order Green functions to the lowest possible level. Equation (25b) is equivalent to the assumption in Section 2 that the thermal averaged z-components of the dressed spins are statistically independent. Equation (24) is equivalent to eq.n (9a) of ref. [7], once noticed that $\lambda_g S = \lambda_g^2 - 2\langle N_g \rangle_T$ represents, in terms of the dressed spins, the same quantity $1 - 2\bar{n} = \sigma$ used therein (recall the second definition (21)).

The self consistent equation determining S follows from calculating the mean value $\langle \langle N_g \rangle \rangle = (\langle \lambda_g^2 \rangle - \langle \lambda_g \rangle \langle S^z \rangle_T) / 2$ and reads (see eq.n (8) in ref. [7] and eq.ns (10)):

$$\frac{1 + \sigma_\lambda^2 - S}{2} = \frac{1}{\mathcal{N}} \int d\omega \text{Tr} \left[\text{Im} \widehat{G}(\omega, S) \right] (e^{\beta\omega} - 1)^{-1}, \quad (26)$$

\mathcal{N} being the total number of spins, $\beta = 1/\kappa T$ and $\hbar = 1$. $\widehat{G}(\omega, S)$ represents the matrix of elements $\widehat{G}_{gf}(\omega, S)$, whose "imaginary" part is defined as [21]:

$$\text{Im} \widehat{G}(\omega, S) = \lim_{\epsilon \rightarrow 0^+} i \left[\widehat{G}(\omega + i\epsilon, S) - \widehat{G}(\omega - i\epsilon, S) \right], \quad (27)$$

in the sense of the distribution theory.

For simplicity, let us split the problem into two parts: on-site disorder without off-site disorder and *vice versa*. The resulting Curie temperatures will be indicated as T_c^{on} and T_c^{off} respectively. Due to the assumed reciprocal independence and to the lowest-order approximation adopted, the two effects can be simply summed up to yield the total effect on T_c . First, we deal with the on-site disorder only. In this case, recalling eq.n (12a), equation (32a) can be put in the form $A\widehat{G} = I$, where the matrix elements of A read, on account of eq.ns (10a):

$$A_{gl} = 2\pi \left[\overbrace{\left\{ \frac{\omega}{S} - 2J_0 \right\} \delta_{lg} + 2J(l-g)}^{A_{gl}^0} \right] - \underbrace{2\pi \frac{\omega}{S} \delta_{lg} (\Delta\lambda_g - \Delta\lambda_g^2 + \dots)}_{\Delta A_{gl}}. \quad (28a)$$

The "unperturbed" matrix A^0 is easily diagonalized on the basis of eigenvectors $|q\rangle$ with g -representation $\langle g|q\rangle = e^{i(gq)}/\sqrt{\mathcal{N}}$ and eigenvalues:

$$a_0(q) = 2\pi \left[\frac{\omega}{S} - 2(J_0 - \hat{J}(q)) \right]; \quad \hat{J}(q) = \sum_f J(f) e^{i(fq)}. \quad (28b)$$

The eigenvalue perturbation is easily found to first order, from the definition (28a):

$$\begin{aligned} \Delta a_1 &= \langle q|\Delta A|q\rangle = -2\pi \frac{\omega}{S} \left[\sum_g \frac{\Delta\lambda_g}{\mathcal{N}} - \sum_g \frac{\Delta\lambda_g^2}{\mathcal{N}} + \dots \right] = \\ &= 2\pi \frac{\omega}{S} \sum_g \frac{\Delta\lambda_g^2}{\mathcal{N}} + \dots, \end{aligned} \quad (29)$$

in which the final expression is obtained from the central limit theorem in the thermodynamic limit. Equation (29) shows that the perturbation is quadratic in the $\Delta\lambda$'s, which leads to include the *second order* perturbation too, for self consistency. We anticipate that this does not change the final result, though the proof is a little bit complicated. The second order perturbation reads, in fact:

$$\begin{aligned} \Delta a_2 &= \sum_{q' \neq q} \frac{\langle q|\Delta A|q'\rangle \langle q'|\Delta A|q\rangle}{a_0(q) - a_0(q')} = \\ &= 2\pi \frac{\omega^2}{S^2 \mathcal{N}^2} \sum_{g,g'} \Delta\lambda_g \Delta\lambda_{g'} \sum_{q' \neq q} \frac{e^{i(q-q')(g'-g)}}{2[\hat{J}(q') - \hat{J}(q)]}. \end{aligned} \quad (30)$$

Following ref. [7], we take the average $\langle a(q) \rangle$, that reads, from eq. ns (29) and (30):

$$\langle a(q) \rangle = a_0(q) + 2\pi \sigma_\lambda^2 \left[\frac{\omega}{S} + \left(\frac{\omega}{S} \right)^2 \Delta_2(q) \right], \quad (31a)$$

with:

$$\Delta_2(q) = \frac{1}{2\mathcal{N}} \sum_{q' \neq q} [\hat{J}(q') - \hat{J}(q)]^{-1}, \quad (31b)$$

At the lowest significant order one sets $A = \sum_q |q; 1\rangle \langle 1; q| / \langle a(q) \rangle$, where $|q; 1\rangle$ is the first-order perturbed eigenvector (not explicitly written here, for brevity). Hence the Green function turns out to be:

$$\begin{aligned} \hat{G} = A^{-1} &= \frac{1}{2\pi(1 + \sigma_\lambda^2)} \sum_q \frac{|q; 1\rangle \langle 1; q|}{[\omega/S - j_0(q) + (\omega/S)^2 \Delta_2(q)]} = \\ &= \frac{1}{2\pi(1 + \sigma_\lambda^2)} \sum_q \frac{|q; 1\rangle \langle 1; q|}{[\omega/S - j_0(q)] [\omega/S - x_-(q)] \Delta_2(q)} \end{aligned} \quad (32a)$$

with

$$j_0(q) = 2 \frac{J_0 - \hat{J}(q)}{1 + \sigma_\lambda^2}, \quad x_-(q) = -\frac{1 + j_0 \Delta_2(q)}{\Delta_2(q)}. \quad (32b)$$

The lower line in eq.n (32a) is obtained by expressing $\langle a \rangle$ (the denominator of the upper line) in terms of its zeroes $x_+ = j_0$ and x_- (second eq.n (32b)), calculated to the lowest order in Δ_2 .

Having expressed \hat{G} as a sum of (double) first order poles in ω/S , equation (27) readily yields

$$\text{Tr} [\text{Im} \hat{G}] = \frac{1}{(1 + \sigma_\lambda^2)} \sum_q \left[\frac{\delta(\omega/S - j_0)}{1 + 2j_0 \Delta_2} + \frac{\delta(\omega/S - x_-)}{(x_- - j_0) \Delta_2} \right]_q. \quad (33)$$

Substituting (33) in eq.n (26), one gets:

$$\begin{aligned} \frac{1 + \sigma_\lambda^2 - S}{2} &= \frac{S}{\mathcal{N}(1 + \sigma_\lambda^2)} \sum_q \left\{ \frac{1}{[e^{\beta S j_0(q)} - 1] [1 + 2j_0(q)]} + \right. \\ &\quad \left. + \frac{1}{\Delta_2(q) [e^{\beta S x_-(q)} - 1] [x_-(q) - j_0(q)]} \right\}, \end{aligned} \quad (34)$$

whose limit $S \rightarrow 0$ gives the equation for T_c^{on} . From eq.ns (32b), and expanding all terms to the lowest order in Δ_2 , equation (34) yields:

$$\begin{aligned} \frac{1 + \sigma_\lambda^2}{2} &= \frac{\kappa T_c^{on}}{\mathcal{N}(1 + \sigma_\lambda^2)} \sum_q \left[\frac{1}{j_0(q)} - \Delta_2(q) \right] = \\ &= \frac{\kappa T_c^{on}}{\mathcal{N}(1 + \sigma_\lambda^2)} \sum_q \frac{1}{j_0(q)}, \end{aligned} \quad (35)$$

since $\sum_q \Delta_2(q) = 0$ for symmetry (eq.n (31b)). As anticipated above, the second-order perturbation term Δ_2 has no influence on the final result eq.n (35). In the absence of on-site disorder, equations (35) and (32b) yield:

$$T_{(\rho, \lambda)}^{-1} = \frac{\kappa}{\mathcal{N}} \sum_q \left[J_0 - \hat{J}(q) \right]^{-1} \quad (36)$$

for the Curie temperature of the average crystal. Then equations (35) and (36) show that the on-site disorder leads to the same increasing factor $T_c^{on}/T_{(\rho, \lambda)} = 1 + \sigma_\lambda^2$ for the Curie temperature of a Heisenberg ferromagnet, as for the semi-classical, Ising-like model.

The effects of the pure off-site disorder can be studied with the same procedure adopted above. The matrix elements A_{gh} now read:

$$\begin{aligned} A_{gh} &= A_{gh}^0 - 4\pi \left[\delta_{gh} \sum_l \frac{\partial J(g-l)}{\partial g_\alpha} \rho_{gl}^\alpha - \frac{\partial J(g-h)}{\partial g_\alpha} \rho_{gh}^\alpha \right] - \\ &- 2\pi \left[\delta_{gh} \sum_l \frac{\partial^2 J(g-l)}{\partial g_\alpha \partial g_{\alpha'}} \rho_{gl}^\alpha \rho_{gl}^{\alpha'} - \frac{\partial^2 J(g-h)}{\partial g_\alpha \partial g_{\alpha'}} \rho_{gh}^\alpha \rho_{gh}^{\alpha'} \right], \end{aligned} \quad (37)$$

where the unperturbed matrix elements A_{gh}^0 are the same as in eq.n (28a) and the sum over repeated α -indices is intended. The first order correction to the unperturbed eigenvalue $a_0(q)$ (eq.n (28b)) is

$$\Delta a_1(q) = \frac{1}{\mathcal{N}} \sum_{gh} e^{iq(h-g)} \underbrace{\langle A_{gh} - A_{gh}^0 \rangle}_{\Delta A_{gh}} = -4\pi\sigma_\rho^2 \left[J_2 - \hat{J}_2(q) \right], \quad (38a)$$

where

$$\hat{J}_2(q) = \frac{1}{2} \sum_f \nabla_D^2 J(D) e^{iq \cdot D}, \quad J_2 = \hat{J}_2(0). \quad (38b)$$

The second order correction is:

$$\Delta a_2(q) = \frac{1}{\mathcal{N}^2} \sum_{q' \neq q} \sum_{g,h,g'h'} \frac{e^{iq(h'-g)+iq'(h-g')}}{a_0(q) - a_0(q')} \langle \Delta A_{gh} \Delta A_{g'h'} \rangle$$

From eq.n (37) and from the relation $\langle \rho_{gh}^\alpha \rho_{g'h'}^{\alpha'} \rangle = \sigma_\rho^2 \delta_{\alpha\alpha'} (\delta_{gg'} \delta_{hh'} - \delta_{gh'} \delta_{hg'})$, one gets:

$$\Delta a_2(q) = \frac{32\pi^2 \sigma_\rho^2}{\mathcal{N}} \sum_{q' \neq q} \frac{\overbrace{J_3^2 + \widehat{J}_3^2(q+q') - \widehat{J}_3^2(q) - \widehat{J}_3^2(q')}^{c(q,q')}}{a_0(q) - a_0(q')}, \quad (39a)$$

with

$$\widehat{J}_3^2(q) = \sum_D [\nabla_D J(D)]^2 e^{iqD}, \quad J_3^2 = \widehat{J}_3^2(0). \quad (39b)$$

The time-transformed Green function

$$\widehat{G} = \sum_q \frac{|q; 1\rangle \langle 1; q|}{a_0(q) + \Delta a_1(q) + \Delta a_2(q)}$$

is now expressed as a sum of *single* poles in ω/s . The equation for T_c readily follows from eq.ns (38), (39) and (28b). At the lowest order in σ_ρ^2 one finally gets:

$$T_c^{oJf} = T_{\langle \rho, \lambda \rangle} [1 + \sigma_\rho^2 (C_+ - C_-)], \quad (40a)$$

with the two constants C_\pm given by:

$$C_+ = \frac{1}{\sum_q [J_0 - \widehat{J}(q)]^{-1}} \sum_q \frac{[J_2 - \widehat{J}_2(q)]}{[J_0 - \widehat{J}(q)]^2}, \quad (40b)$$

$$C_- = \frac{1}{\mathcal{N} \sum_q [J_0 - \widehat{J}(q)]^{-1}} \sum_{q,q'} \frac{c(q,q') [2J_0 - \widehat{J}(q) - \widehat{J}(q')]}{[J_0 - \widehat{J}(q)]^2 [J_0 - \widehat{J}(q')]^2}. \quad (40c)$$

The positivity of the two terms C_\pm is not "universal". However, from the definition of $c(q, q')$ in eq.n (39a), it follows that $C_\pm > 0$ if $\widehat{J}(q)$ and $\widehat{J}_3^2(q)$ are positive and decreasing with increasing argument, which is the standard case in the ferromagnetic regime. In conclusion, the Curie temperature of a Heisenberg ferromagnet, including both chemical and structural disorder, turns out to be:

$$T_c = T_{\langle\rho,\lambda\rangle} [1 + \sigma_\lambda^2 + \sigma_\rho^2 (C_+ - C_-)] , \quad (41)$$

to the lowest significant order in the random fluctuations. The overall sign of $C_+ - C_-$ depends on the coupling function $J(r-r')$ in a complicated way, and cannot be determined by simple arguments. For Heisenberg-like systems, the enhancement or depression of T_c due to the structural disorder is, thereby, model-dependent.

4 Comparison with other MF theories

A comparison of the preceding results can be made with the MF theories developed in refs [11, 7], that assume the interaction energy $U(r, r')$ as an overall random variable. In this representation, the disorder effects are those produced by the energy fluctuations *about the mean value* $\langle U \rangle$ that determines the average crystal and, accordingly, the reference Curie temperature $T_{\langle U \rangle}$. Since there is no rescaling of the interacting variables, one is left with the calculation of the mean value $\langle\langle s \rangle\rangle$ of the "naked" spins. Let us first consider the Ising-like systems. In this case it is easy to see from ref. [11] that $T_c = T_{\langle U \rangle}$, and the disorder effects simply result in a *depression* of the magnetization, in the close proximity of the Curie temperature:

$$\langle\langle s \rangle\rangle \propto \sqrt{1 - \frac{T}{T_{\langle U \rangle}}} (1 - \delta^2) , \quad (42)$$

where δ is proportional to the fluctuations of the interaction energy. In the present model, one has $\langle\langle s \rangle\rangle = \langle\lambda^{-1}\rangle\langle\langle S \rangle\rangle = (1 + \sigma_\lambda^2) \langle\langle S \rangle\rangle$, according to eq.ns (10) (the lowest order approximation is intended), and $\sigma_x^2 \propto (1 - T/T_c)$ (eq.ns (13)). Hence, setting $T = T_{\langle\rho,\lambda\rangle}$ in eq.n (14b) and after a suitable rearrangement of terms in eq.ns (13), (14b), one gets:

$$\langle\langle s \rangle\rangle \propto \sqrt{1 - \frac{T}{T_c}} (1 - \delta^2) , \quad (43a)$$

$$\delta^2 = 2\sigma_\lambda^2 \left(\frac{1 + 2J_1^2/J_0^2}{1 - J_1^2/J_0^2} \right) + \frac{3}{2}\sigma_\rho^2 \left(\frac{J_3^2/J_0^2}{1 - J_1^2/J_0^2} \right) . \quad (43b)$$

As can be seen, the random fluctuations of the coupling energy U , resulting from σ_λ^2 and σ_ρ^2 , tend to depress $\langle\langle s \rangle\rangle$ close to the Curie temperature, as in eq.n (42).

At this stage, it is instructive expressing $T_{\langle U \rangle}$ (eq.n (42)) in terms of the present model. First, we calculate the mean value and the standard deviation of the interaction energy according to eq.ns (1) and (2):

$$\langle U(r, r') \rangle = \int dP_\rho dP_\lambda U(r, r') = -J(f - f') - \frac{\sigma_\rho^2}{2} \nabla_f^2 J(f - f'), \quad (44a)$$

$$\sigma_U^2 = \sigma_\rho^2 [\nabla_f J(f - f')]^2 + 2\sigma_\lambda^2 J(f - f'). \quad (44b)$$

Since $T_{\langle U \rangle}$ is the Curie temperature corresponding to the average crystal with interaction energy eq.n (44a), one easily gets:

$$\left. \begin{aligned} T_{\langle U \rangle} &= T_{\langle \rho, \lambda \rangle} (1 + J_2 \sigma_\rho^2) \\ T_c &= T_{\langle U \rangle} + \sigma_\lambda^2 T_{\langle \rho, \lambda \rangle} \end{aligned} \right\} \text{(Ising)} \quad (45)$$

in which $T_{\langle \rho, \lambda \rangle}$ (eq.n (14a)) is the reference Curie temperature in the chemical-structural disorder representation, and the lower line follows from eq.n (15). It is not difficult to perform the same calculation for the Heisenberg-like systems too. From eq.ns (44) and (41), it follows that

$$\left. \begin{aligned} T_{\langle U \rangle} &= T_{\langle \rho, \lambda \rangle} (1 + \sigma_\rho^2 C_+) \\ T_c &= T_{\langle U \rangle} - \sigma_\rho^2 C_- T_{\langle \rho, \lambda \rangle} + \sigma_\lambda^2 T_{\langle \rho, \lambda \rangle} \end{aligned} \right\} \text{(Heisenberg)}. \quad (46)$$

In the absence of *chemical* disorder ($\sigma_\lambda^2 = 0$), equations (45) and (46) recover the results of ref.s [11, 7] that the Curie temperature is not affected by the random fluctuations of the interaction energy *about its mean value*, in Ising-like systems (eq.n (45)), and decreases linearly with σ_U^2 in Heisenberg-like systems (eq.n (46)). In fact, the term $J_2 \sigma_\rho^2$ comes from eq.n (44a), and the term $-\sigma_\rho^2 C_- T_{\langle \rho, \lambda \rangle}$ comes from eq.n (44b), i.e. right from σ_U (eq.n (40c)).

The main point of the preceding arguments is that, passing from the chemical-structural representation to the one adopted in ref.s [7, 11] (in which the unique random variable is U itself), the positive terms $J_2 \sigma_\rho^2$ and $T_{\langle \rho, \lambda \rangle} \sigma_\rho^2 C_+$, due to the structural disorder, seemingly disappear, since they are incorporated in $T_{\langle U \rangle}$ (i.e. in a different average crystal). In contrast, the increasing effect of the *chemical* disorder on T_c cannot be removed by a redefinition of the average crystal, i.e. by replacing $T_{\langle \rho, \lambda \rangle}$ with $T_{\langle U \rangle}$. This shows that the model interaction eq.n (1) and the one adopted in ref.s [7, 11] cannot be mapped one into another, except in the absence of chemical disorder. At this stage, it should be clear that speaking about a Curie temperature increasing (or decreasing) with increasing disorder is misleading, unless one defines exactly which representation of the disorder has been adopted.

5 Applications

As mentioned in Section 1, the model interaction eq.n (1) is an ideal expression in which the spin-spin coupling can be exactly factorized in a part $J(r-r')$, depending only on the positions of the spins (structural disorder), and a part $\lambda_r \lambda_{r'}$, accounting for the characteristic of the spins themselves (chemical disorder). The simplest application is certainly on *ferroelectric* systems. In this case the "spins" are actually atomic scale displacements of charges, generating electric dipoles, whose intensity is determined by the Born effective charge Z_r^* , that can be related, after suitable rescaling, to the on-site parameter λ_r . The dipole-dipole coupling $J(r-r')$ is usually split into a nearest-neighbor contribute, strongly dependent on the local symmetries, plus a long-range term $\propto |r-r'|^{-3}$ [22]. Of course, the present model applies to *magnetic* dipoles too, whose interaction energy is usually small, compared to the exchange interaction. However, there are cases in which this is not true [23]. A theoretical model for perovskite ferroelectrics, leading to an increase of T_c has been formulated by Bokov [10], by calculating the total polarization as the sum of single-cell contributions, each characterized by a local T_c , whose fluctuations reflect the different cationic content of the cell. An experimental support to the validity of eq.n (15) has been obtained right for *ferroelectric* perovskites, by Sinclair and Attfield [5]. The measured T_c of ATiO₃-systems (with A a cation) is shown to increase linearly with the square standard deviation σ_A^2 of the A-radius size, whose random fluctuations are obtained by the binary cationic mixture $A = \text{Ba}_{1-x}\text{Mg}_x$, and the changes of σ_A^2 are controlled by the relative concentration x . In this case, it is reasonable to think of a direct influence of the cationic disorder on the Born effective charge, or on other *local* quantities determining the dipole intensity. This would result in what we call the *chemical* disorder, whose enhancing effect on T_c is common to Ising-like and Heisenberg-like systems.

The application of eq.n (1) to the exchange magnetic interactions is less immediate. As a typical example, let us deal with a substitutional random alloy, each site of which can be occupied by an orbital ψ_α , with probability p_α . In this case the true exchange energy between two spins with relative position $D = r - r'$ reads:

$$\begin{aligned}
 U_{true}(r, r') &= -e^2 \int \int \frac{dr_1 dr_2}{|r_1 - r_2|} \times \\
 &\quad \times \psi_{\alpha_r}(r_1) \psi_{\alpha_{r'}}^*(r_1 - D) \psi_{\alpha_{r'}}(r_2 - D) \psi_{\alpha_r}^*(r_2) = \\
 &= U_{true}(\alpha_r, \alpha_{r'}; D) .
 \end{aligned} \tag{47}$$

Since the on-site features are displayed by the two orbitals $\psi_{\alpha_r}, \psi_{\alpha_{r'}}$, it is clear that no exact factorization is possible. However, in view of a

qualitative account of the on-site *vs* off-site disorder effects, one can replace U_{true} with a form like eq.n (1), for an appropriate choice of $J(D)$ and λ_r . In particular, the quantities

$$J(D) = - \sum_{\alpha, \alpha'} p_{\alpha} p_{\alpha'} U_{true}(\alpha, \alpha'; D) \quad (48a)$$

$$\begin{aligned} \lambda_r &= \frac{\sum_{\alpha'} p_{\alpha'} \int U_{true}(\alpha_r, \alpha'; D) dD}{\int J(D) dD} = \\ &= \frac{\sum_{\alpha'} p_{\alpha'} \int U_{true}(\alpha', \alpha_r; D) dD}{\int J(D) dD} \end{aligned} \quad (48b)$$

define, respectively, the mean dependence of the exchange energy on the relative position, and on the on-site orbital (note that $\langle \lambda_r \rangle = 1$). In this case, $U(r, r') = -\lambda_r \lambda_{r'} J(D)$ reproduces the statistical properties of U_{true} *modulo* the coupling of the random variables' fluctuations. Hence, the use of eq.ns (48) is especially suitable in a MF approximation, aiming to achieve a guess of the relative importance of the chemical and structural disorder.

Recent theoretical works have stressed the importance of the *thermal* disorder for a correct interpretation of the magnetic properties. In ref. [15, 16], the coupling between thermal fluctuations and itinerant electrons is argued to yield a crucial contribute to the magnetization, especially in the transition between ballistic and diffusive regime. In ref. [24] the effects of the thermal expansivity on the magnetization are shown to be non negligible in some cases. It is worthwhile mentioning that the disordered crystal model and eq.n (2) have a straightforward application to the thermal disorder effects in an otherwise perfect ferromagnetic crystal. In this case, in fact, the fluctuations of the distance $|r - r'|$, described by the random variable ρ , are of pure thermal origin. For high enough temperature T , the probability distribution P_{ρ} is Gaussian with square standard deviation $\sigma_{\rho}^2 = \kappa T / M \Omega_D^2$, where M is the atomic mass (for monoatomic systems), and Ω_D is comparable to the Debye frequency. In the reasonable hypothesis that the spin variables are fast enough to allow for the application of the Born-Oppenheimer approximation, equation (40a) can be used to calculate the resulting (structural) disorder effect on the Curie temperature:

$$T_c^{off} = T_{\langle \rho \rangle} \left[1 + \frac{\kappa T_{\langle \rho \rangle}}{M \Omega_D^2} (C_+ - C_-) \right], \quad (49)$$

$T_{\langle \rho \rangle}$ being the Curie temperature of the *rigid* crystal.

6 Conclusions

In the present work the disorder effects on the Curie temperature, due to the chemical and structural disorder, have been studied separately, by assuming a suitably factorized form of the spin interactions (eq.n (1)). It is shown that the chemical (on site) disorder leads to distinguish between spins s_g and "dressed" spins $S_g = \lambda_g s_g$. In the realm of the mean field approximation, it has been argued that the better approximation is assuming $\langle\langle S_g \rangle\rangle$ site-independent, and calculating the dressed magnetization $\propto \langle\langle S \rangle\rangle$. If necessary, one may set $\langle\langle s \rangle\rangle = \langle\lambda^{-1}\rangle\langle\langle S \rangle\rangle$. Following this line, it has been shown in Sections 2 , 3 that the chemical disorder enhances T_c , by a term proportional to the square standard deviation σ_λ^2 , both in Ising-like and in Heisenberg-like systems. The structural (off-site) disorder enhances in turn the T_c of the Ising-like systems, but contributes two terms $\pm\sigma_\rho^2 C_\pm$, with opposite sign, to the T_c of the Heisenberg-like systems. The overall effect, enhancement or depression, is model-dependent. Since $-\sigma_\rho^2 C_-$ is specific of the Heisenberg-like systems with structural disorder, one may argue that the *delocalization* driven by the spin waves is the unique responsible of the negative sign.

Special emphasis is given (Section 4) to the representation of the disorder, by comparing the present model with other MF theories [11, 7], in which the random variable is the interaction energy $U(r, r')$ itself. It is shown that the structural disorder provides a representation equivalent to the one in ref.s [11, 7], while the chemical disorder does not. This argument calls attention on the necessity of specifying the disorder representation adopted, in order that the enhancement or depression of the Curie temperature is defined unambiguously.

Supports to the results in Sections 2 , 3 have been found in experimental data and other theoretical models referring to perovskite *ferroelectrics* [5, 9, 10], to which the factorization (1) applies directly. In ferromagnets, a comparison with experiments is less immediate and, at present, not significant, for two related reasons. First, most of the experimental works on ferromagnets are concerned on the modifications of T_c induced by changes of some controlled *average* parameters (pressure, alloy/defect concentration, etc.). The effects of the random fluctuations about those average values (what we mean for "disorder effects") are indeed more difficult to be observed. Second, the current theoretical approaches usually deal with the interaction energy $U(r, r')$ as with an overall random variable and no clear separation is made between structural and chemical part [11, 7]. Indeed, the factorization (1) is not exactly feasible, if the chemical-structural features are nested in an *exchange* integral, as it is the case of ferromagnets. However, the approximate method suggested in Section 5 for factorizing the two contributions in the exchange interactions too, could be of some

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8 use for triggering the experimental and theoretical work on the different
9 effects of the two basic elements of disorder, chemical and structural, even
10 in ferromagnetic materials.

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