Magnetic Properties of Two-Dimensional (2D) Heisenberg Lattices as Good Candidates for Spintronic Junctions

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***Abstract* — In this article we briefly recall a theoretical treatment previously published [1] and concerning the magnetic properties of 2D square lattices composed of $(2N+1)^2$ classical spins isotropically coupled between first-nearest neighbors (i.e., showing Heisenberg couplings). Indeed these layers are good candidates for spintronic junctions. In the thermodynamic limit ($N \to +\infty$), we recall that (i) a very simple closed-form expression may be derived for the zero-field partition function $Z_N(0)$, (ii) the spin correlation vanishes in the zero-field limit i.e., there is no remnant magnetization, except at T=0 K; (iii) the spin-spin correlation is described by a correlation path confined inside a correlation domain (Theorem 1). As a result a general closed-form expression may be respectively derived for the spin-spin correlation between any two lattice sites (Theorem 2) and for the susceptibility, without any approximation. We finally test previous experimental fits and we show that the use of a truncated expansion for the susceptibility was totally justified.**

***Index Terms* — spintronics, classical spins, Heisenberg couplings, magnetic properties, quantum theory**

I. INTRODUCTION

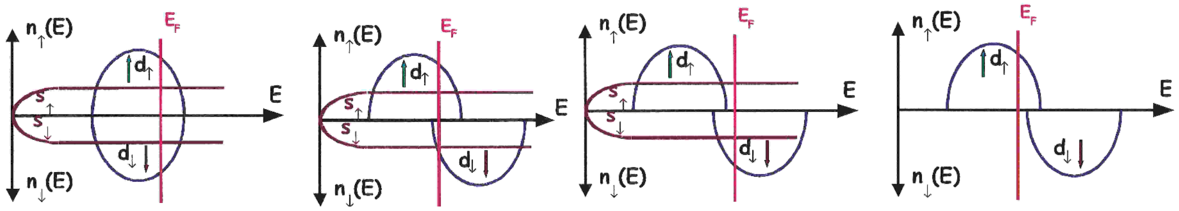
From a practical point of view, thin magnetic layers play an important role in many areas of technology. Namely, in the field of spintronics, these layers may appear at the interface between different semiconductors showing or not magnetic properties [2]. Indeed, in a magnetic material, spin scattering mechanisms are closely dependent on the energy level E occupied by the external electrons respectively labelled s, p or d as well as on their polarization "up" (↑) or "down" (↓). In Fig.1 we have summarized the various situations which intervene and allow one to understand the nature of the spin current passing through a junction, notably at the Fermi level EF. Thus, if n(EF) is the electron density at the Fermi level, we have for (i) a nonferromagne-tic metal $n_{s\uparrow}(E_F) = n_{s\downarrow}(E_F)$ and $n_{d\uparrow}(E_F) = n_{d\downarrow}(E_F)$ whereas (ii) for a weak ferromagnet $n_{s\uparrow}(E_F) = n_{s\downarrow}(E_F)$ but $n_{d\uparrow}(E_F) \neq n_{d\downarrow}(E_F)$. As a result the corresponding spin current is composed of electrons s↑, s↓, d↑ and d↓ but we have □↑≠□↓ for the resistivities. Spintronics exploits this asymmetry of conduction so that there are two channels of conduction. (iii) In the case of a strong ferromagnet, the current is composed of electrons s↑, s↓ and d↓ , exclusively, whereas for (iv) a "semimetal" (generally an oxide such as CrO2, Fe3O4, …, a metallic alloy such as NiMnSb or a semiconductor such as GaMnAs) only electrons d↑ play a role. If we define the polarization P at the Fermi level as:

$$P = \frac{|n_\uparrow(E_F) - n_\downarrow(E_F)|}{n_\uparrow(E_F) + n_\downarrow(E_F)} \tag{1}$$

we shall have a full polarization (100%) in cases (iii) with electrons d↓ and in case (iv) with electrons d↑.

As a result, the study of the magnetic properties of three-dimensional (3D) compounds composed of 3d ions is of the highest importance. In addition they constitute an intermediate step for building up 3D artificial magnets whose structure may be imposed (like for magnetic grains used in nanotechnologies) and are characterized by local spins of high quantum number i.e., spin momenta characterized by a spin quantum number plainty greater or equal to 5/2.

Two-dimensional (2D) magnetic layers are also very important because they may be used at the interface of blocks constituting spintronic junctions. This is the reason for



Case (i)
Nonferromagnetic Metal

Case (ii)
Weak Ferromagnet

Case (iii)
Strong Ferromagnet

Case (iv)
Semimetal

Fig.1. Comparison of the spin densities at the Fermi level for different cases of magnetic properties (the $s_\uparrow$ and $s_\downarrow$ densities have been omitted in case (iv) for clarity)

which the study of their magnetic properties has drawn such an attention in addition to the fact that physics in two dimen-sions is very different, notably for interpreting the fractional quantum Hall effect [3].

In previous papers [4] we published a treatment concerning the 2D square lattices composed of (2N+1)2 classical spins (for instance, ions Mn2+ and Fe3+ characterized by a spin quantum number 5/2) isotropically coupled between nearest neighbors (i.e., showing Heisenberg couplings). However it was based upon an approximation that we shall recall. These layers are good candidates for spintronic junctions. Indeed, when dealing with a ferromagnet, the resistivity strongly depends on the relative orientation of the spin current and the local magnetization. When dealing with an antiferromagnet, the magnetization is plainly weaker and the resistivity will be quasi independent from the local magnetization.

In the thermodynamic limit (N→+∞), we recall that (i) a very simple closed-form expression may be derived for the zero-field partition function ZN(0), (ii) the spin correlation vanishes in the zero-field limit i.e., there is no remnant magnetization, except at T=0 K; (iii) the spin-spin correlation is described by a correlation path confined inside a correlation domain (Theorem 1). As a result a general closed-form expression may be respectively derived for the spin-spin correlation between any two lattice sites (Theorem 2) and the susceptibility, without any approximation. We finally test previous experimental fits and we show that the use of a truncated expansion for the susceptibility was totally justified [4], [5]. We shall see in conclusion of this paper that, in fact, the approximation used was fully justified except in a very sharp temperature domain closed to absolute zero (the critical temperature TC).

II. THE ZERO-FIELD PARTITION FUNCTION, THE SPIN CORRELATIONS AND THE SUSCEPTIBILITY

1. *Generalities*

In Magnetism the static and/or dynamic physical quantities of highest interest are the magnetization, the susceptibility and the correlation length. All these parameters share a common property: their respective definitions involve the presence of spin correlations. In this article we shall exclusively focus on the static properties of the *susceptibility* χ, in the zero-field limit. Generally it is more convenient to reduce the susceptibility χ to the susceptibility per lattice site $\chi_{i,j}$. Thus we may define the susceptibility per lattice site as:

$$\chi_{i,j} = \beta \sum_{k} \sum_{k'} G_{i,j} G_{i+k,j+k'} \Gamma_{k,k'} \qquad (2)$$

where $G_{u,u'}$ is the Landé factor directly expressed in $\mu_B/\hbar$ unit and characterizing each classical spin momentum:

$$G_{i,j} = G \quad \text{if } i+j \text{ is even or zero,}$$
$$G_{i,j} = G' \quad \text{if } i+j \text{ is odd ,} \qquad (3)$$

and where $\Gamma_{k,k'}$ is the *correlation function*:

$$\Gamma_{k,k'} = <\boldsymbol{S}_{i,j}.\boldsymbol{S}_{i+k,j+k'}> - <\boldsymbol{S}_{i,j}><\boldsymbol{S}_{i+k,j+k'}> . \qquad (4)$$

In the previous equation, the bracket notation <…> means that we deal with a thermodynamic average. In other words, if we consider a lattice wrapped on a torus, characterized by a square unit cell and composed of (2N+1)2 sites, each one being the carrier of a classical spin Si,j, we may define the correlation between any two spins as:

$$<\boldsymbol{S}_{i,j}.\boldsymbol{S}_{i+k,j+k'}> = \frac{1}{Z_N(0)} \int d\boldsymbol{S}_{-N,-N} \ldots \int \boldsymbol{S}_{i,j} d\boldsymbol{S}_{i,j} \ldots \int \boldsymbol{S}_{i+k,j+k'} d\boldsymbol{S}_{i+k,j+k'} \ldots \int d\boldsymbol{S}_{N,N} \exp\left(-\beta \sum_{i=-N}^{N} \sum_{j=-N}^{N} H_{i,j}^{ex} \right) \qquad (5)$$

where $Z_N(0)$ is the zero-field partition function derived from the numerator of (5) by replacing the absent spin $\boldsymbol{S}_{i,j}$ or $\boldsymbol{S}_{i+k,j+k'}$ by the vector (1,1,1). $d\boldsymbol{S}$ is the elementary surface swept by the extremity of spin $\boldsymbol{S}(\theta,\varphi)$ i.e. $d\boldsymbol{S} = \cos\theta d\theta d\varphi$, in spherical co-ordinates. $H_{i,j}^{ex}$ is the exchange Hamiltonian

$$H_{i,j}^{ex} = (J_1 \boldsymbol{S}_{i,j+1} + J_2 \boldsymbol{S}_{i+1,j}) \boldsymbol{S}_{i,j} \qquad (6)$$

In the previous equation we recall that J_1 and J_2 refer to the exchange interaction between nearest neighbors belonging to the horizontal lines and vertical rows of the lattice, respectively. In addition $J_i>0$ (respectively, $J_i<0$, with i=1,2) denotes an antiferromagnetic (respectively, ferromagnetic) coupling. $<\boldsymbol{S}_{i,j}.\boldsymbol{S}_{i+k,j+k'}>$ is called the *spin-spin correla-tion* whereas $<\boldsymbol{S}_u>$, with u=(i,j) or (i+k,j+k'), is the *spin correlation.* $<\boldsymbol{S}_u>$ may be directly derived from (5) by replacing the absent spin $\boldsymbol{S}_{i,j}$ or $\boldsymbol{S}_{i+k,j+k'}$ in $<\boldsymbol{S}_{i,j}.\boldsymbol{S}_{i+k,j+k'}>$ by the vector (1,1,1). From a physical point of view this correlation $<\boldsymbol{S}_{i,j}.\boldsymbol{S}_{i+k,j+k'}>$ will describe the state of cor-relation between any two spins located at sites (i,j) and (i+k,j+k'). As for $<\boldsymbol{S}_u>$, with u=(i,j) or (i+k,j+k'), it is directly linked with the magnetization per site. In the zero-field limit to which we restrict the present study, it is nothing but the remnant magnetization per site. In addition, as we deal with isotropic (Heisenberg) couplings, we have the following properties:

$$<S_{i,j}^{v}.S_{i+k,j+k'}^{v}> = \frac{1}{3}<\boldsymbol{S}_{i,j}.\boldsymbol{S}_{i+k,j+k'}> , \quad v = x, y \text{ or } z,$$

$$<S_u^v> = \frac{1}{3}<\boldsymbol{S}_u> , \qquad (6)$$

$$\boldsymbol{S}_u = S_u^x \boldsymbol{e}_x + S_u^y \boldsymbol{e}_y + S_u^z \boldsymbol{e}_z , \; u = (i,j) \text{ or } (i+k,j+k'),$$

from which we immediately derive for the correlation func-tion:

$$\Gamma_{k,k'}^{v} = \frac{1}{3}\Gamma_{k,k'} , \quad v = x, y \text{ or } z \qquad (7)$$

Finally we may define the *self spin-spin correlation* $<(S_u^v)^2>$, with v=x, y or z. We have $<\boldsymbol{S}^2>=1$ due to the fact that the classical spin is considered as a *unit vector*. Consequently, as we deal with isotropic spin-spin couplings, we may write:

$$<(S_u^x)^2> = <(S_u^y)^2> = <(S_u^z)^2> = \frac{1}{3},$$

$$\chi_{i,j}^{x} = \chi_{i,j}^{y} = \chi_{i,j}^{z} = \frac{\chi_{i,j}}{3} . \qquad (8)$$

From now we shall consider the reference site as (i,j)=(0,0). Under these conditions, the expression of the susceptibility per square unit cell and averaged per lattice site may be finally written as:

$$\chi = \frac{1}{4}\left(\chi^z_{0,0} + \chi^z_{0,1} + \chi^z_{1,0} + \chi^z_{1,1}\right), \tag{9}$$

In [1] we have seen that, because of the presence of classical spin moments, all the operators $H^{ex}_{i,j}$ commute and the exponential factor appearing in the integrand of (5) may be written:

$$\exp\left(-\beta \sum_{i=-N}^{N} \sum_{j=-N}^{N} H^{ex}_{i,j}\right) = \prod_{i=-N}^{N} \prod_{j=-N}^{N} \exp\left(-\beta H^{ex}_{i,j}\right). \tag{10}$$

Thus, the particular nature of $H^{ex}_{i,j}$ given by (6) allows one to separate the contributions corresponding to the exchange coupling involving classical spins belonging to the same horizontal line i of the layer (i.e., $\boldsymbol{S}_{i,j-1}$, $\boldsymbol{S}_{i,j+1}$ and $\boldsymbol{S}_{i,j}$) or to the same vertical row j (i.e., $\boldsymbol{S}_{i-1,j}$, $\boldsymbol{S}_{i+1,j}$ and $\boldsymbol{S}_{i,j}$) [1]. Thus, for each of the four contributions (one per bond connected to the site (i,j) carrying the spin $\boldsymbol{S}_{i,j}$), we have to expand a term

such as $\exp(-A\boldsymbol{S}_1.\boldsymbol{S}_2)$ where A is βJ_1 or βJ_2 (the classical spins $\boldsymbol{S}_1$ and $\boldsymbol{S}_2$ being considered as unit vectors). If we call $\Theta_{1,2}$ the angle between vectors $\boldsymbol{S}_1$ and $\boldsymbol{S}_2$, respectively characterized by the couples of angular variables (θ_1,φ_1) and (θ_2,φ_2), it is possible to expand the operator $\exp(-A\cos\Theta_{1,2})$ on the infinite basis of spherical harmonics which are eigenfunctions of the angular part of the Laplacian operator on the sphere of unit radius S2:

$$\exp\left(-A\cos\Theta_{1,2}\right) =$$

$$4\pi \sum_{\ell=0}^{+\infty} \left(\frac{\pi}{2A}\right)^{1/2} \mathrm{I}_{\ell+1/2}(-A) \sum_{m=-\ell}^{+\ell} Y^*_{\ell,m}(\boldsymbol{S}_1) Y_{\ell,m}(\boldsymbol{S}_2). \tag{11}$$

In the previous equation, the $\mathrm{I}_{\ell+1/2}(-A)$'s are modified Bessel functions of the first kind. If we set:

$$\lambda_\ell(-\beta j) = \left(\frac{\pi}{2\beta j}\right)^{1/2} \mathrm{I}_{\ell+1/2}(-\beta j), \quad j = J_1, J_2, \tag{12}$$

each operator $\exp\left(-\beta H^{ex}_{i,j}\right)$ may be notably expanded on the basis of eigenfunctions (the spherical harmonics), whereas the □□'s are nothing but the associated eigenvalues. As Oz is the axis of quantization in the spin momentum space, we shall exclusively focus on the z-z spin-spin correlation or on the z spin-correlation. In the most general case we have:

$$< S^z_{i,j}.S^z_{i+k,j+k'} > = \frac{(4\pi)^{2(2N+1)^2}}{Z_N(0)} \sum_{\ell_{N,-N}=0}^{+\infty} \lambda_{\ell_{N,-N}}(-\beta J_1) \sum_{\ell'_{N,-N}=0}^{+\infty} \lambda_{\ell'_{N,-N}}(-\beta J_2) \times \ldots$$

$$\times \sum_{\ell_{-N,N-1}=0}^{+\infty} \lambda_{\ell_{-N,N-1}}(-\beta J_1) \sum_{m_{N,-N}=-\ell_{N,-N}}^{+\ell_{N,-N}} \; \sum_{m'_{N,-N}=-\ell'_{N,-N}}^{+\ell'_{N,-N}} \ldots \sum_{m_{-N,N-1}=-\ell_{-N,N-1}}^{+\ell_{-N,N-1}} \prod_{k_1=-N}^{N} \prod_{k_2=-N}^{N} F'_{k_1,k_2} \tag{13}$$

At this step, let us note that, due to the previous remarks, $< \boldsymbol{S}_{i,j}.\boldsymbol{S}_{i+k,j+k'} >$ (as well as ZN(0) and all the derived ther-modynamic functions) appears as a characteristic polyno-mial expressed by means of eigenfunctions (the spherical harmonics) and associated eigenvalues (the □□'s) of the La-placian operator. F'_{k_1,k_2} is the following current integral

$$F'_{k_1,k_2} = \int d\boldsymbol{S}_{k_1,k_2} X_{k_1,k_2} Y_{\ell'_{k_1+1,k_2},m'_{k_1+1,k_2}}(\boldsymbol{S}_{k_1,k_2}) Y_{\ell_{k_1,k_2-1},m_{k_1,k_2-1}}(\boldsymbol{S}_{k_1,k_2}) Y^*_{\ell_{k_1,k_2},m_{k_1,k_2}}(\boldsymbol{S}_{k_1,k_2}) Y^*_{\ell'_{k_1,k_2},m'_{k_1,k_2}}(\boldsymbol{S}_{k_1,k_2}), \tag{14}$$

with

$$X_{k_1,k_2} = \cos\theta_{k_1,k_2} \quad \text{for } k_1 = i,\ k_2 = j \ \underline{\text{or}}\ k_1 = i + k,\ k_2 = j + k' \quad (< S^z_{i,j} > \ \underline{\text{or}} < S^z_{i+k,j+k'} >), \tag{15a}$$

$$X_{k_1,k_2} = \cos\theta_{k_1,k_2} \quad \text{for } k_1 = i,\ k_2 = j \ \underline{\text{and}}\ k_1 = i + k,\ k_2 = j + k' \quad (< S^z_{i,j}.S^z_{i+k,j+k'} >), \tag{15b}$$

$$X_{k_1,k_2} = 1 \quad \text{for } k_1 \neq i,\ k_2 \neq j \ \underline{\text{or/and}}\ k_1 \neq i + k,\ k_2 \neq j + k'. \tag{15c}$$

When $X_{k_1,k_2} = 1$, we have $F'_{k_1,k_2} = F_{k_1,k_2}$. This latter integral which has been calculated in [1] for expressing the zero-field partition function ZN(0) may be written as:

$$F_{k_1,k_2} = \frac{1}{4\pi}\left[(2\ell'_{k_1+1,k_2}+1)(2\ell_{k_1,k_2-1}+1)(2\ell_{k_1,k_2}+1)(2\ell'_{k_1,k_2}+1)\right]^{1/2} \sum_{L_{k_1,k_2}=L_<}^{L_>} \frac{1}{2L_{k_1,k_2}+1} \times$$

$$\times \sum_{M_{k_1,k_2}=-L_{k_1,k_2}}^{+L_{k_1,k_2}} C^{L_{k_1,k_2}\ 0}_{\ell'_{k_1+1,k_2}\ 0\ \ell_{k_1,k_2-1}\ 0}\, C^{L_{k_1,k_2}\ M_{k_1,k_2}}_{\ell'_{k_1+1,k_2}\ m'_{k_1+1,k_2}\ \ell_{k_1,k_2-1}\ m_{k_1,k_2-1}}\, C^{L_{k_1,k_2}\ 0}_{\ell_{k_1,k_2}\ 0\ \ell'_{k_1,k_2}\ 0}\, C^{L_{k_1,k_2}\ M_{k_1,k_2}}_{\ell_{k_1,k_2}\ m_{k_1,k_2}\ \ell'_{k_1,k_2}\ m'_{k_1,k_2}} \tag{16}$$

In the previous equation $C^{\ell_3\ m_3}_{\ell_1\ m_1\ \ell_2\ m_2}$ is a Clebsch-Gordan (C.G.) coefficient [6]. The C.G. coefficients appearing in (17) (with $M_{k_1,k_2} \neq 0$ or $M_{k_1,k_2} = 0$) do not vanish if the triangular inequalities $\left|\ell_{k_1,k_2} - \ell'_{k_1,k_2}\right| \leq L_{k_1,k_2} \leq \ell_{k_1,k_2} + \ell'_{k_1,k_2}$ and $\left|\ell'_{k_1+1,k_2} - \ell_{k_1,k_2-1}\right| \leq L_{k_1,k_2} \leq \ell_{k_1,k_2-1} + \ell'_{k_1+1,k_2}$ are fulfilled, respectively. As a result, we must have $L_<$=max($\left|\ell'_{k_1+1,k_2} - \ell_{k_1,k_2-1}\right|, \left|\ell_{k_1,k_2} - \ell'_{k_1,k_2}\right|$) and $L_>$= min($\ell_{k_1,k_2-1} + \ell'_{k_1+1,k_2}$, $\ell_{k_1,k_2} + \ell'_{k_1,k_2}$).

2. Calculation of $Z_N(0)$

The calculation of the zero-field partition function $Z_N(0)$ involves that of each current integral $F_{i,j}$ (*cf.* (17)). Whatever the finite or infinite lattice size, the non-vanishing condition of $F_{i,j}$ is mainly due to that of C.G. coefficients for the in-sites. The first C.G. coefficient $C^{L_{i,j}\ M_{i,j}}_{\ell'_{i+1,j}\ m'_{i+1,j}\ \ell_{i,j-1}\ m_{i,j-1}}$ will not vanish if $M_{i,j}=m'_{i+1,j}+m_{i,j-1}$ whereas for the second one $C^{L_{i,j}\ M_{i,j}}_{\ell_{i,j}\ m_{i,j}\ \ell'_{i,j}\ m'_{i,j}}$ we have $M_{i,j}=m_{i,j}+m'_{i,j}$ [6] so that we finally derive $(2N+1)^2$ equations (one per lattice site) such as:

$$m_{i,j-1}+m'_{i+1,j}-m_{i,j}-m'_{i,j}=0 \quad (SRm). \qquad (17)$$

This is the first selection rule labelled from now SRm: it exclusively concerns the various coefficients $m_{i,j}$ and $m'_{i,j}$ characterizing each site (i,j). The SRm relation is unique and temperature-independent; (ii) due to the fact that the φ-part of the $F_{i,j}$-integrand (exclusively depending on the m's and m"s) reduces to unity, $F_{i,j}$ is a purely real number.

The second non-vanishing condition of C.G. coefficients appearing in each current integral $F_{i,j}$ (cf (17)) concerns the positive (or zero) integers $\ell_{i,j}$ and $\ell'_{i,j}$ intervening in each radial factor of the characteristic polynomial. In addition to the triangular inequalities $|\ell_{i,j}-\ell'_{i,j}|\leq L_{i,j}\leq \ell_{i,j}+\ell'_{i,j}$ and $|\ell_{i,j-1}-\ell'_{i+1,j}|\leq L_{i,j}\leq \ell_{i,j-1}+\ell'_{i+1,j}$ respectively followed by the C.G. coefficients $C^{L_{i,j}\ M_{i,j}}_{\ell_{i,j}\ m_{i,j}\ \ell'_{i,j}\ m'_{i,j}}$ and $C^{L_{i,j}\ M_{i,j}}_{\ell'_{i+1,j}\ m'_{i+1,j}\ \ell_{i,j-1}\ m_{i,j-1}}$ (with $M_{i,j}\neq 0$ or $M_{i,j}=0$), we have a more restrictive vanishing condition when the involved mi,j's and m'i,j's are replaced by zero as it clearly appears in (17) [6]:

$$C^{\ell_3\ 0}_{\ell_1\ 0\ \ell_2\ 0}=0, \qquad \text{if } \ell_1+\ell_2+\ell_3=2g+1,$$

$$C^{\ell_3\ 0}_{\ell_1\ 0\ \ell_2\ 0}=(-1)^{g-\ell_3}\sqrt{2\ell_3+1}\ K, \ \text{if } \ell_1+\ell_2+\ell_3=2g, \qquad (18)$$

where K is a coefficient which remains unchanged under the permutation of integers ℓ_1, ℓ_2 and ℓ_3. As a result $C^{L_{i,j}\ 0}_{\ell_{i,j}\ 0\ \ell'_{i,j}\ 0}$ will not vanish if $\ell_{i,j}+\ell'_{i,j}+L_{i,j}=2A_{i,j}\geq 0$ whereas, for $C^{L_{i,j}\ 0}_{\ell'_{i+1,j}\ 0\ \ell_{i,j-1}\ 0}$, we must have $\ell_{i,j-1}+\ell'_{i+1,j}+L_{i,j}=2A'_{i,j}\geq 0$.

If we sum the two previous equations concerning ℓ and ℓ', we have $(2N+1)^2$ equations (one per lattice site) such as:

$$\ell_{i,j-1}+\ell'_{i+1,j}+\ell_{i,j}+\ell'_{i,j}=2g_{i,j}\,,\ g_{i,j}=A_{i,j}+A'_{i,j}-L_{i,j}\geq 0 \quad (SR\ell 1) \qquad (19)$$

or by assuming the difference:

$$\ell_{i,j-1}+\ell'_{i+1,j}-\ell_{i,j}-\ell'_{i,j}=2g'_{i,j}\,,\ g'_{i,j}=A'_{i,j}-A_{i,j} \quad (SR\ell 2) \qquad (20)$$

(or equivalently $\ell_{i,j}+\ell'_{i,j}-\ell_{i,j-1}-\ell'_{i+1,j}=2g''_{i,j}$, with $g''_{i,j}=-g'_{i,j}$).

Thus, the complete determination of couples (□i,j,mi,j) for each lattice site (i,j) will allow the full determination of the closed-form expression of ZN(0). It is achieved owing to two properties: (i) using principles of invariance which must be respected by the expression of $Z_N(0)$; (ii) using the spin lat-tice symmetries.

(i) *Owing to the first property of invariance, the closed-form expression obtained for the zero-field partition function* $Z_N(0)$ *must be invariant under the permutation of the exchange energies* J_1 *and* J_2 *(diagonal or D-symmetry). The second property of invariance imposes that the expression of* $Z_N(0)$ *must be independent of the bond orientation.*

(ii) We essentially wish to determine $Z_N(0)$ in the thermodynamic limit ($N\to+\infty$) i.e., in the physical case of an infinite lattice. As a result it is easier to wrap the lattice on a torus because there are more symmetry elements than for a 2D plane lattice. However, in the physical case $N\to+\infty$, $Z_N(0)$ must be similar in both cases. For both situations, we deal with two elements of symmetry (*step 1*): the horizontal and vertical medians (mirror planes $\mathcal{M}_1$ and $\mathcal{M}_2$). *The effect of such mirrors is to transform a spherical harmonic into another conjugated one and vice versa*. Thus we must have $F_{i,j}=F_{-i,j}^{*}$ (symmetry with respect to the horizontal median - *HM*-symmetry - or mirror $\mathcal{M}_1$) and $F_{i,j}=F_{i,-j}^{*}$ (symmetry with respect to the vertical median - *VM*-symmetry - or mirror $\mathcal{M}_2$). As all the integrals $F_{i,j}$ are real due to the *SRm* condition (*cf* (18)) we finally have $F_{i,j}=F_{-i,j}$ (mirror $\mathcal{M}_1$) and $F_{i,j}=F_{i,-j}$ (mirror $\mathcal{M}_2$). It allows one to derive specific relations between the involved coefficients m and ℓ. More details are given in [1]. In *Step 2* we now use a new element of symmetry: the torus is characterized by an axis of revolution Δ. As a result it means that mirror $\mathcal{M}_2$ which contains this axis can rotate around it. It then allows one to show that two consecutive vertical lines are constituted of bonds characterized by the same couple of values (ℓ'_i,m'_j).

Finally, in *Step 3*, the *D*-symmetry operation (exchange of indices 1 and 2) permits to derive that $m_i=m'_j$ and $\ell_i=\ell'_j$ if $i=j$. As we have just shown that all the bonds of the vertical lines of the torus are characterized by the same couple (ℓ'_j,m'_j), we derive that all the horizontal lines as well as all the vertical ones are characterized by the same couple $(\ell_i,m_i)=(\ell'_j,m'_j)$ or equivalently

$$m_{i,j}=m'_{i,j}=m\ ,\ \ \ell_{i,j}=\ell'_{i,j}=\ell\ \ \forall\,(i,j)\in\text{Torus}. \qquad (21)$$

This result is in perfect agreement with the geometrical properties of a toroidal environment, for each lattice site. In summary the property followed by coefficients □ (respectively, m) is similar to the one encountered in the case of a finite chain showing cyclic conditions.

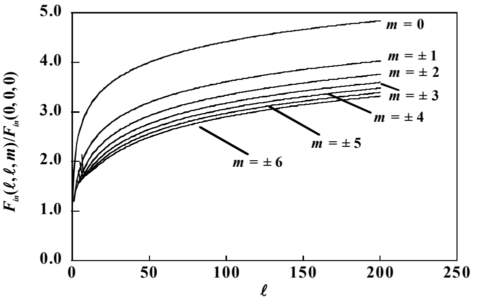


Fig.2. Plot of the ratio $F_{in}(\ell,\ell,m)/F_{in}(0,0,0)$ *vs* ℓ for various values of m

Consequently we may write the general expression of the zero-field partition function for a finite torus:

$$Z_N^{Torus}(0)=(4\pi)^{2(2N+1)^2}\times$$

$$\times\sum_{\ell=0}^{+\infty}\sum_{m=-\ell}^{+\ell}\left[\lambda_\ell(-\beta J_1)\lambda_\ell(-\beta J_2)F_{in}(\ell,\ell,m)\right]^{(2N+1)^2} \quad (22)$$

where the function $\lambda_\ell(-\beta J_i)$, with i=1,2, is given by (13) and the current integral $F_{in}(\ell,\ell,m)$ may be directly written from (17) i.e.,

$$F_{in}(\ell,\ell,m)=\frac{(2\ell+1)^2}{4\pi}\sum_{L=0}^{2\ell}\frac{1}{2L+1}\left[C_{\ell\ 0\ \ell\ 0}^{L\ 0}\,C_{\ell\ m\ \ell\ m}^{L\ 2m}\right]^2 . \quad (23)$$

In Fig.2 we have reported the ratio $F_{in}(\ell,\ell,m)/F_{in}(0,0,0)$ (with $F_{in}(0,0,0)=1/4\pi$) *vs* ℓ for various m-values such as $|m|\le\ell$. We immediately observe that this ratio rapidly decreases for increasing $|m|$-values, for a given ℓ-value. We always have $F_{in}(\ell,\ell,|m|)<F_{in}(\ell,\ell,0)$. In addition, in a further numerical study achieved for m=0 but not reported here by lack of place, we have shown that $F_{in}(\ell_i,\ell_j,0)$ decreases for $\ell_j<\ell_i$. As a result, when $N\to+\infty$, only the integral $F_{in}(\ell,\ell,0)$ belonging to the generic term $\left[F_{in}(\ell,\ell,m)\right]^{(2N+1)^2}\approx\left[F_{in}(\ell,\ell,m)\right]^{4N^2}$ prevails so that the value m=0 is selected. Thus, as in the 1D-case with cyclic boundary conditions, when the lattice wrapped on a torus becomes infinite, the edge effects become negligible. As a result the zero-field partition function associated with the torus of infinite curvature radii and given by (23) may be written:

$$Z_N(0)=(4\pi)^{8N^2}\sum_{\ell=0}^{+\infty}\left[\lambda_\ell(-\beta J_1)\lambda_\ell(-\beta J_2)F_{\ell,\ell}\right]^{4N^2},$$

as $N\to+\infty$ (24)

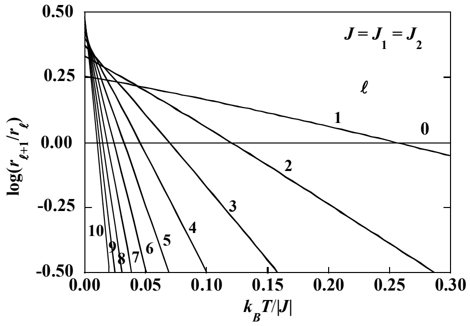


Fig.3. Thermal variations of the ratio $\log(r_{\ell+1}/r_\ell)$ for various values of ℓ where r_ℓ is defined by (27)

where the integral $F_{\ell,\ell}$ is the new simplified expression of integral $F_{in}(\ell,\ell,m)$ given by (24), with here m=0 i.e.,

$$F_{\ell,\ell}=F_{in}(\ell,\ell,0)=\frac{(2\ell+1)^2}{4\pi}\sum_{L=0}^{2\ell}\frac{1}{2L+1}\left[C_{\ell\ 0\ \ell\ 0}^{L\ 0}\right]^4 . \quad (25)$$

The question is now the following one: is it necessary to keep all the terms in the □-expansion of ZN(0)? In order to answer to this important question which will condition the respective expressions of the spin-spin correlations and the susceptibility we must study the following ratio r_ℓ:

$$r_\ell=\frac{\lambda_\ell(-\beta J_1)\lambda_\ell(-\beta J_2)}{\lambda_0(-\beta J_1)\lambda_0(-\beta J_2)}\frac{F_{in}(\ell,\ell,0)}{F_{in}(0,0,0)} . \quad (26)$$

The numerical study restricted to the case $J=J_1=J_2$ for sake of simplicity has been detailed in [1] but the reasoning may be easily extended to the general case $J_1\neq J_2$. As a result, we briefly report the thermal behavior of the ratio $r_{\ell+1}/r_\ell$ where r_ℓ is given by (27), for various ℓ-values (see Fig.3). In the very low-temperature domain we may then observe a succession of *crossovers*, each crossover being characterized by a specific temperature called *crossover temperature* T_{CO}. For instance, for the reduced temperature $k_BT/|J|\ge0.255$, $\lambda_0(-\beta J)$ appears in the dominant term of the characteristic polynomial whereas, for $0.255\ge k_BT/|J|\ge 0.043$, $\lambda_1(-\beta J)$ belongs to the dominant one etc... In that case the crossover temperature corresponding to the transition between the regimes respectively characterized by ℓ=0 and ℓ=1 is labelled $T_{CO_{0,1}}$. This study will be very useful later when fitting experimental susceptibilities.

3. Calculation of $<S_u^z>$ and $<S_{i,j}^z.S_{i+k,j+k'}^z>$

The calculation of the numerator of the spin correlation $<S_u^z>$ and the spin-spin correlation $<S_{i,j}^z.S_{i+k,j+k'}^z>$ is strictly similar to that of $Z_N(0)$. It is given by (14) in which we have $X_{k_1,k_2}=1$ except at sites (i,j) or ($i+k,j+k'$) where we use the following transform:

$$\cos\theta_{k_1,k_2}Y_{\ell_{k_1,k_2},m_{k_1,k_2}}(\boldsymbol{S}_{k_1,k_2})=C_{\ell_{k_1,k_2}+1}Y_{\ell_{k_1,k_2}+1,m_{k_1,k_2}}(\boldsymbol{S}_{k_1,k_2})+C_{\ell_{k_1,k_2}-1}Y_{\ell_{k_1,k_2}-1,m_{k_1,k_2}}(\boldsymbol{S}_{k_1,k_2}) \quad (27)$$

with:

$$C_{\ell_{k_1,k_2}+1}=\left[\frac{(\ell_{k_1,k_2}+1+m_{k_1,k_2})(\ell_{k_1,k_2}+1-m_{k_1,k_2})}{(2\ell_{k_1,k_2}+1)(2\ell_{k_1,k_2}+3)}\right]^{1/2},\quad C_{\ell_{k_1,k_2}-1}=\left[\frac{(\ell_{k_1,k_2}+m_{k_1,k_2})(\ell_{k_1,k_2}-m_{k_1,k_2})}{(2\ell_{k_1,k_2}+1)(2\ell_{k_1,k_2}-1)}\right]^{1/2} \quad (28)$$

The transform law given by (28) does not change coefficients m and m' so that the selection rule SRm given by (18) is unchanged when calculating the numerator of $<S_u^z>$ and $<S_{i,j}^z.S_{i+k,j+k'}^z>$. When applying (28) at site (i,j) and/or at site ($i+k,j+k'$) in (14) we deal with a new integral F'_{k_1,k_2} which may be written:

$$F'_{k_1,k_2}=C_{\ell_{k_1,k_2}+1}\widetilde{F}_{\ell_{k_1,k_2}+1}+C_{\ell_{k_1,k_2}-1}\widetilde{F}_{\ell_{k_1,k_2}-1} \quad (29)$$

with:

$$\widetilde{F}_{\ell_{k_1,k_2}+\varepsilon}=\int d\boldsymbol{S}_{k_1,k_2}Y_{\ell'_{k_1+1,k_2},m'_{k_1+1,k_2}}(\boldsymbol{S}_{k_1,k_2})Y_{\ell_{k_1,k_2-1},m_{k_1,k_2-1}}(\boldsymbol{S}_{k_1,k_2})Y^*_{\ell_{k_1,k_2}+\varepsilon,m_{k_1,k_2}}(\boldsymbol{S}_{k_1,k_2})Y^*_{\ell'_{k_1,k_2},m'_{k_1,k_2}}(\boldsymbol{S}_{k_1,k_2}),\ \ \varepsilon=\pm1, \quad (30)$$

if the transform is applied to $Y^{*}_{\ell_{k_1,k_2},m_{k_1,k_2}}(\boldsymbol{S}_{k_1,k_2})$, for instance. This integral may be expressed like integral F_{k_1,k_2} given by (17). It also contains C.G. coefficients. When studying $\widetilde{F}_{\ell_{k_1,k_2}+\varepsilon}$ in the numerator of $<S^z_u>$ we have previously shown that the involved C.G. coefficients cannot vanish simultaneously [1]. As a result

$$<S^z_{i,j}>=0,\ \ <S^z_{i+k,j+k'}>=0,$$

$$\Gamma^z_{k,k'}=\ <S^z_{i,j}.S^z_{i+k,j+k'}>\ \text{for } T>0\text{ K}. \tag{31}$$

Of course, when T=0 K exactly, we have: $|<S^z_{i,j}>|=1$. *This result rigorously proves that the critical temperature is absolute zero* i.e., T_C=0 K.

When calculating the numerator of $<S^z_{i,j}.S^z_{i+k,j+k'}>$, we have two integrals F'_{k_1,k_2}, one at site (*i,j*) and one at site (*i+k,j+k'*). We now have four contributions, each of them respectively containing the products $\widetilde{F}_{l_{i,j}+1}\widetilde{F}_{l_{i+k,j+k'}+1}$, $\widetilde{F}_{l_{i,j}+1}\widetilde{F}_{l_{i+k,j+k'}-1}$, $\widetilde{F}_{l_{i,j}-1}\widetilde{F}_{l_{i+k,j+k'}+1}$ and $\widetilde{F}_{l_{i,j}-1}\widetilde{F}_{l_{i+k,j+k'}-1}$, with *l*=ℓ or *l*=ℓ', each one being similar to that one appearing in the calculation of $Z_N(0)$. The detailed calculation of the numerator of $<S^z_{i,j}.S^z_{i+k,j+k'}>$ is given in [1]. Below we just report the main results by lack of place.

<u>Theorem 1</u>: For calculating the numerator of the spin-spin correlation $<S^z_{i,j}.S^z_{i+k,j+k'}>$, one must take into account two domains: a correlation domain which is a rectangle of vertices (i,j), (i,j+k'), (i+k,j+k') and (i+k,j) within which all the correlation paths are confined, and a remaining domain called wing domain. In both domains we have m=m$_0$ (for a finite lattice) and m=0 (for an infinite lattice). In addition all the bonds of the wing domain are characterized by the same coefficient ℓ_0, including the bonds linked with the correlation domain.

<u>Theorem 2</u>: All the correlation paths show the same length inside the correlation domain which is the shortest possible one in agreement with Feynman's principle. They involve the same number of horizontal and vertical bonds than the horizontal and vertical sides of the correlation rectangle, for the 2D square lattice. The corresponding spin-spin correla-tion $<S^z_{i,j}.S^z_{i+k,j+k'}>$ is then expressed owing to (33)-(36).

$$<S^z_{0,0}.S^z_{k,k'}>=\frac{1}{Z_N(0)}\sum_{\ell=0}^{+\infty}\left[\lambda_\ell(-\beta J_1)\lambda_\ell(-\beta J_2)F_{\ell,\ell}\right]^{4N^2}\left[X_{\ell+1}+(1-\delta_{\ell,0})X_{\ell-1}\right],\ k>0,\ k'>0,\ \text{as } N\to+\infty \tag{32}$$

where $\delta_{\ell,0}$ is the Dirac function and with:

$$X_{\ell+\varepsilon}=\left(C_{\ell+\varepsilon}\right)^2\frac{F_{\ell,\ell+\varepsilon}}{F_{\ell,\ell}}\left[\frac{\lambda_{\ell+\varepsilon}(-\beta J_1)}{\lambda_\ell(-\beta J_1)}\frac{F_{\ell,\ell+\varepsilon}}{F_{\ell,\ell}}\right]^{k'}\left[\frac{\lambda_{\ell+\varepsilon}(-\beta J_2)}{\lambda_\ell(-\beta J_2)}\frac{F_{\ell,\ell+\varepsilon}}{F_{\ell,\ell}}\right]^{k},\ k\geq 0,\ k'\geq 0,\ \varepsilon=\pm 1, \tag{33}$$

$$C_{\ell+1}=\frac{\ell+1}{\sqrt{(2\ell+1)(2\ell+3)}},\ \ C_{\ell-1}=\frac{\ell}{\sqrt{(2\ell+1)(2\ell-1)}}. \tag{34}$$

$$F_{\ell,\ell+\varepsilon}=\widetilde{F}_{\ell+\varepsilon}=\frac{1}{4\pi}(2\ell+1)(2\ell+2\varepsilon+1)\sum_{L=0}^{\min(2\ell,2\ell+2\varepsilon)}\frac{1}{2L+1}\left[C^{L\ \ 0}_{\ell\ \ 0\ \ \ell\ \ 0}\,C^{L\ \ 0}_{\ell+\varepsilon\ \ 0\ \ \ell+\varepsilon\ \ 0}\right]^2,\ F_{0,\varepsilon}=1,\ \ \varepsilon=\pm 1. \tag{35}$$

4. Calculation of the susceptibility

As we now know the closed-form expression of the spin-spin correlation (*cf* (33)-(36)), it then possible to express the susceptibility owing to (2). We have:

$$\chi=\frac{1}{Z_N(0)}\sum_{\ell=0}^{+\infty}\left[\lambda_\ell(-\beta J_1)\lambda_\ell(-\beta J_2)F_{\ell,\ell}\right]^{4N^2}\left[\chi_{\ell+1}+(1-\delta_{\ell,0})\chi_{\ell-1}\right],\ \text{as } N\to+\infty \tag{36}$$

with:

$$\chi_{\ell+\varepsilon}=\frac{\beta}{2}\left(C_{\ell+\varepsilon}\right)^2\frac{F_{\ell,\ell+\varepsilon}}{F_{\ell,\ell}}\frac{(G^2+G'^2)W_{1,\ell+\varepsilon}+2GG'W_{2,\ell+\varepsilon}}{W_{3,\ell+\varepsilon}},\ \varepsilon=\pm 1, \tag{37}$$

$$W_{1,\ell+\varepsilon}=[1+(u_{1,\ell+\varepsilon})^2][1+(u_{2,\ell+\varepsilon})^2]+4u_{1,\ell+\varepsilon}u_{2,\ell+\varepsilon},\ \ W_{2,\ell+\varepsilon}=2[u_{1,\ell+\varepsilon}(1+(u_{2,\ell+\varepsilon})^2)+u_{2,\ell+\varepsilon}(1+(u_{1,\ell+\varepsilon})^2)] \tag{38}$$

$$W_{3,\ell+\varepsilon}=[1-(u_{1,\ell+\varepsilon})^2][1-(u_{2,\ell+\varepsilon})^2],\ \ u_{i,\ell+\varepsilon}=\frac{\lambda_{\ell+\varepsilon}(-\beta J_i)}{\lambda_\ell(-\beta J_i)}\frac{F_{\ell,\ell+\varepsilon}}{F_{\ell,\ell}},\ i=1,2 \tag{39}$$

We observe that, in the generic expression of the susceptibility given by (37), we deal with a □-series, as for ZN(0). Furthermore, if we examine the numerator, it also appears the current term $\left[\lambda_\ell(-\beta J_1)\lambda_\ell(-\beta J_2)F_{\ell,\ell}\right]^{4N^2}$ coming from ZN(0). This term has been studied in [1], in the particular case J1=J2. We have seen (cf Fig.3) that, there is a succession of crossovers, each crossover being characterized by a specific temperature called crossover temperature TCO. Thus, for the reduced temperature kBT/|J|≥0.255,□0̃(□J) appears in the dominant term of the characteristic polynomial whereas, for 0.255≥kBT/|J|≥0.043,□1̃(□J) belongs to the dominant one etc... In addition, when the temperature is cooling down, near absolute zero, we have a succession of closer and closer crossovers (due to the fact that the various crossover temperatures TCO are closer and closer). In other words, all the eigenvalues, characterized by an increasing □-value, successively play a role. But, when T≈0 K, i.e., near the critical point, all these eigenvalues intervene due to the fact that the crossover temperatures vanish with ℓ.

Fits of experimental results

We do not achieved here the low-temperature study of the susceptibility by lack of place. But, as noted for the study of the zero-field partition function $Z_N(0)$, we may assert that the closed-form expression, previously obtained for the susceptibility by restricting the various ℓ-expansions to $\ell=0$ [4], remains valid here for reduced temperatures such as $k_BT/|J|\geq 0.255$ and $T\approx 0$K, near the critical point $T_C=0$ K. The other terms characterized by $\ell>0$ in (37) will only play a role below 0.255, as explained for $Z_N(0)$ in [1]. More particularly, this role will be enhanced in the reduced temperature range [0–ε',0.255[, with ε'→0.

From a practical point of view, in order to see if an experimental fit is valid or not by restricting the ℓ-expansion of the susceptibility given by (37) to $\ell=0$, one must compare the reduced Néel température $k_BT_N/|J|$ to 0.255 (if we deal with 2 different exchange energies J_1 and J_2 we shall have to compare $k_BT_N/\sqrt{|J_1J_2|}$ to 0.255).

In a previous paper [5], we fitted the experimental susceptibilities measured for the three compounds [{$MnL_2(N_3)_2$}$_n$], with L=DENA (compound **1**), 4acpy (compound **2**) and minc (compound **3**), with the following meaning for the ligand abbreviation L: L=DENA (diethyl-nicotinamide), 4acpy (4-acetylpyridine) and minc (methyl isonicotinate). In these new family of compounds, the co-ordination polyhedra of the Mn atoms show a common apex, and the 4.2 Å Mn–Mn intralayer distance is twice the Mn–F bond distance in the well-known prototype K_2MnF_4. As a result we deal with quasi-2D lattices composed of classical spins (S=5/2) i.e., Mn atoms, each one occupying the summit of a square unit cell. Each centrosymmetric Mn atom is octahedrally co-ordinated to four azido bridges and ligands L in *trans* arrangement. In addition, from a magnetic point of view, these compounds are characterized by isotropic (Heisenberg) couplings between first-nearest spin neighbors.

These fits have been achieved through the closed-form expression of the susceptibility given by (37) and restricted to the first term of the ℓ-expansion i.e., $\ell=0$. There are reported again in Fig.4.

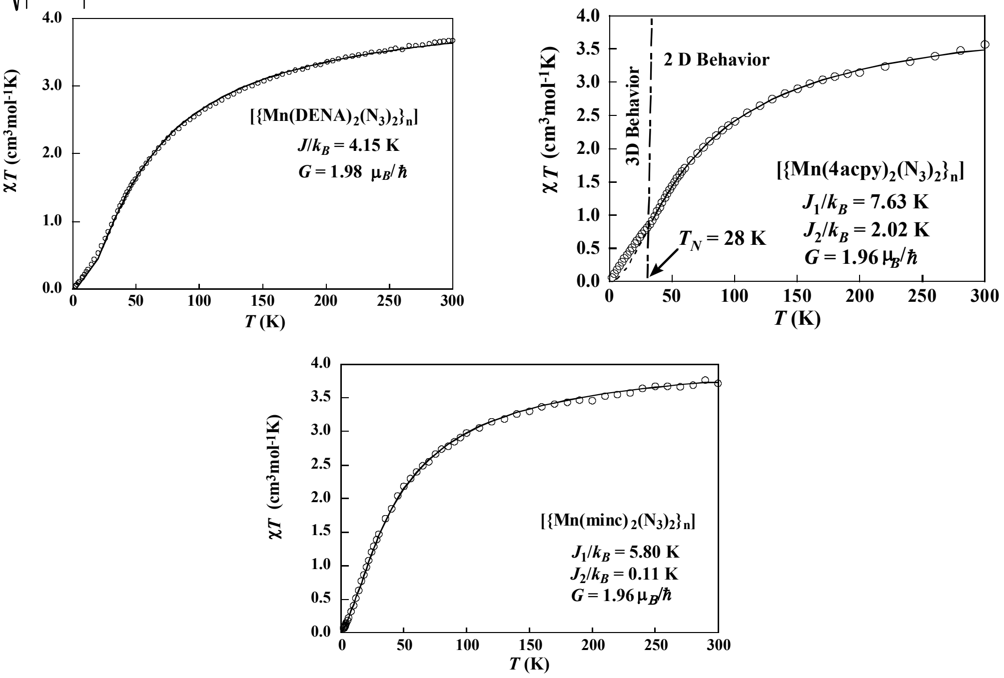


Fig. 4. Fit of the experimental susceptibility χ (open circles) for a polycrystalline sample of the antiferromagnet [{$MnL_2(N_3)_2$}$_n$] characterized by a 2D classical Heisenberg square lattice with the theoretical expression of the susceptibility χ given by (37-40) reduced to the first term $\ell=0$ of the ℓ-expansion

In Table I, we compare the reduced Néel température $k_BT_N/\sqrt{|J_1J_2|}$ to 0.255, for compounds **1** (L=DENA), **2** (L=4acpy) and **3** (L=minc). We immediately observe that, for the 3 compounds, we always have $k_BT_N/\sqrt{|J_1J_2|}>$ 0.255. As a result, these numerical tests totally validate the previous fits *a posteriori*.

TABLE I
COMPARISON OF THE NÉEL REDUCED TEMPERATURE FOR COMPOUNDS 1, 2 AND 3 PREVIOUSLY FITTED [5] WITH RESPECT TO 0.255

L	DENA	4acpy	minc
J_1/k_B (K)	4.15 ± 0.02	7.63 ± 0.15	5.80 ± 0.07
J_2/k_B (K)	4.15 ± 0.02	2.02 ± 0.11	$0.11 \pm 0.00_3$
Néel Temperature T_N (K)	~ 2.0	28.0	~ 2.0
Reduced Néel Temperature $k_BT_N/\sqrt{\lvert J_1J_2\rvert}$	0.48_2	7.13_2	2.23_8

III. CONCLUSION

In this article we have recalled the general method used in [1] for deriving the characteristic polynomial associated with the zero-field partition function ZN(0) of a finite lattice wrapped on a torus. The spin correlation vanishes if T□0 but remains finite at T=0 K, thus proving that absolute zero *plays the role of critical temperature*.

We have seen again that, for calculating the numerator of the spin-spin correlation $< S_{i,j}^z . S_{i+k,j+k'}^z >$, we have to take into account two domains: a *correlation domain* which is a rectangle of vertices (*i,j*), (*i,j+k'*), (*i+k,j+k'*) and (*i+k,j*) within which all the correlation paths are confined, and a remaining domain called *wing domain*. In both domains we have $m = m_0$ (for a finite lattice) and $m = 0$ (for an infinite lattice). In addition all the bonds of the wing domain are characterized by the same coefficient ℓ_0, including the bonds linked with the correlation domain (Theorem 1). Then we have also recalled that all the correlation paths show the same length inside the correlation domain which is the shortest possible one in agreement with Feynman's principle. They respectively involve the same number of horizontal and vertical bonds than the horizontal and vertical sides of the correlation rectangle, for the 2D square lattice (Theorem 2).

The closed-form expression of the spin-spin correlation has allowed to derive the susceptibility in the important physical case of an infinite torus which also behaves as an infinite 2D plane lattice. By restricting the corresponding ℓ-expansion to the first term $\ell = 0$, we have retrieved a previous result [4]. In this article, we have shown that this approximation remains valid for reduced temperatures such as $k_B T / |J| \geq 0.255$ and $T \approx 0$ K, near the critical point $T_C = 0$ K. The other terms characterized by $\ell > 0$ in (37) only play a role below 0.255, as explained for $Z_N(0)$ in [1]. More particularly, this role will be enhanced in the reduced temperature range $[0 - \varepsilon', 0.255[$, with $\varepsilon' \to 0$, so that one may expect interesting crossover phenomena, near absolute zero, in the critical domain.

Finally we have verified that previous experimental fits [5] were valid while using a ℓ-expansion of the susceptibility reduced to the first term $\ell = 0$. In this purpose, we have compared the reduced Néel température $k_B T_N / \sqrt{|J_1 J_2|}$ to 0.255, for three compounds previously studied. In all cases we always have $k_B T_N / \sqrt{|J_1 J_2|} > 0.255$. As a result, these numerical tests totally validate the previous fits *a posteriori*. They finally allow one to give a good test of the present theoretical model developed without any approximation.

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