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Magnetism of 2*d* Heisenberg classical square lattices: theory *vs* experiments

Jacques Curély[*,1] **and Janis Kliava**[2]

[1] Université Bordeaux 1, 351 Cours de la Libération, 33405 Talence Cedex, France
[2] LOMA, Université Bordeaux 1, 351 Cours de la Libération, 33405 Talence Cedex, France

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* Corresponding author: e-mail jacques.curely@u-bordeaux1.fr, Phone: +33 540 002 603, Fax: +33 540 006 970

In this article, we exclusively focus on the low-temperature behaviors of 2*d* square lattices composed of $(2N+1)^2$ classical spins with isotropic couplings between first-nearest neighbors (Heisenberg couplings), in the thermodynamic limit ($N \to +\infty$). After briefly recalling the theoretical closed-form expressions derived for (i) the zero-field partition function $Z_N(0)$, (ii) the spin-spin correlation between any two lattice sites, (iii) the correlation length and (iv) the static susceptibility, we build up a diagram characterized by three low-temperature magnetic phases. Moreover we show that the behaviors of these physical quantities as well as the diagram are in perfect agreement with the corresponding ones derived using a renormalization method. Finally we give criterions allowing to directly determine the magnetic phases characterizing 2*d* magnetic compounds described by our microscopic model. An experimental test is given for illustrating this theoretical study. It allows one to obtain a perfect fit of the susceptibility of $[\{Mn(DENA)_2(N_3)_2\}_n]$ (DENA is the ligand diethylnicotinamide).

1 Introduction Thin magnetic layers play an important role in many areas of technology because they may show a great variety of very different physical properties. Namely, in the field of spintronics, these layers can appear at the interface between different semiconductors showing or not magnetic order. Two-dimensional (2*d*) antiferromagnets such as La_2CuO_4 turn out to be high-temperature superconductors when properly doped [1]. Magnetic layers also constitute an intermediate step for building up 3*d* artificial magnets whose structure may be imposed (like for magnetic grains used in nanotechnologies) and are characterized by local spins of high quantum number.

As a result the theoretical modelling is of the highest interest, notably the 2*d* Heisenberg model [1]. The starting point of this model consists in considering an exchange Hamiltonian in which the spins are isotropically coupled. Thus the magnetic properties of La_2CuO_4 may be described by this model. The lattice composed of spins ½ showing isotropic couplings between first-nearest neighbors is characterized by a square unit cell. Chakravarty *et al.* [1] have shown that the long-wave length excitations and low-energy properties are well-described by a mapping to a 2*d*-classical Heisenberg magnet because all the effects of quantum fluctuations can be resorbed by means of adapted renormalizations of the coupling constants. In other words the spins ½ may be replaced by classical spins i.e., spins characterized by a spin quantum number $S \geq 5/2$.

In previous papers [2] one of us gave a first treatment for the 2*d* square lattice composed of classical spins showing Heisenberg couplings (isotropic couplings between first-nearest neighbors). More recently, one of us published a couple of papers [3] in which we rigorously established, for the first time, the closed-form expressions of the zero-field partition function and the spin-spin correlation, respectively. In this article, after recalling these important results we describe low-temperature behaviors of the correlation length and the static susceptibility derived from the spin-spin correlations for infinite lattices. This leads to the determination of a diagram including three magnetic phases. Moreover we show that all the behaviors are in perfect agreement with the corresponding ones derived by using the renormalization method. An experimental test is given for illustrating this theoretical study.

2 Theoretical background

2.1 Generalities The starting point of the 2*d* classical Heisenberg model consists in expressing the general Hamiltonian describing a lattice characterized by a square unit cell and wrapped on a torus so that it contains $(2N+1)^2$ sites, each one being the carrier of a classical spin $\boldsymbol{S}_{i,j}$:

$$H = \sum_{i=-N}^{N} \sum_{j=-N}^{N} \left(H_{i,j}^{ex} + H_{i,j}^{mag}\right), \tag{1}$$

with

$$H_{i,j}^{ex} = (J_1 \boldsymbol{S}_{i,j+1} + J_2 \boldsymbol{S}_{i+1,j}) \boldsymbol{S}_{i,j}, \tag{2}$$

$$H_{i,j}^{mag} = -G_{i,j} S_{i,j}^z B \ , \tag{3}$$

where

$$G_{i,j} = G \quad \text{if } i+j \text{ is even or zero,}$$
$$G_{i,j} = G' \quad \text{if } i+j \text{ is odd.} \tag{4}$$

In (2) 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. $G_{i,j}$ is the Landé factor characterizing each spin $\boldsymbol{S}_{i,j}$ and expressed in $\mu_B/\hbar$ unit, where μ_B is Bohr's magneton and $\hbar=h/2\pi$, h being Planck's constant. Now one may wonder why we consider a lattice wrapped on a torus. At first sight, one can guess that it is due to the fact that a torus possesses more symmetry elements than a plane lattice. But, *in* the infinite limit (N→+∞), we previously showed [3] that these two types of lattices are characterized by the same partition function Z_N. As a result, all the thermodynamic functions derived from Z_N are similar.

In the present article we exclusively focus on physical quantities expressed in the zero-magnetic field limit. In that case the zero-field partition function $Z_N(0)$ is given by

$$Z_N(0) = \int d\boldsymbol{S}_{-N,-N} \ldots \int d\boldsymbol{S}_{i,j} \ldots \int d\boldsymbol{S}_{N,N} \exp\left(-\beta \sum_{i=-N}^{N} \sum_{j=-N}^{N} H_{i,j}^{ex}\right) \tag{5}$$

where $\beta=1/k_BT$. The magnetic susceptibility $\chi_{i,j}$ per lattice site and the correlation length ξ are defined as

$$\chi_{i,j} = \beta \sum_k \sum_{k'} G_{i,j} G_{i+k,j+k'} \Gamma_{k,k'} \ , \tag{6}$$

$$\xi = \left(\frac{\sum_k \sum_{k'} (k^2 + k'^2) \left|\Gamma_{k,k'}\right|}{\sum_k \sum_{k'} \left|\Gamma_{k,k'}\right|} \right)^{1/2} , \tag{7}$$

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

$$\Gamma_{k,k'} = <\boldsymbol{S}_{i,j}.\boldsymbol{S}_{i+k,j+k'}> - <\boldsymbol{S}_{i,j}><\boldsymbol{S}_{i+k,j+k'}> . \tag{8}$$

In the previous equation, the bracket notation <**…**> means that we deal with a thermodynamic average. As a result we may define the spin-spin correlation between any two spins as:

$$<\boldsymbol{S}_{i,j}.\boldsymbol{S}_{i+k,j+k'}> = \frac{1}{Z_N(0)} \int d\boldsymbol{S}_{-N,-N} \ldots \int \boldsymbol{S}_{i,j} d\boldsymbol{S}_{i,j} \ldots \int \boldsymbol{S}_{i+k,j+k'} d\boldsymbol{S}_{i+k,j+k'} \ldots \int d\boldsymbol{S}_{N,N} \exp\left(-\beta \sum_{i=-N}^{N} \sum_{j=-N}^{N} H_{i,j}^{ex}\right). \tag{9}$$

The spin correlation $<\boldsymbol{S}_u>$, with $u=(i,j)$ or $(i+k,j+k')$, can be simply derived from (9) by replacing $\boldsymbol{S}_{i,j}$ or $\boldsymbol{S}_{i+k,j+k'}$ by unity.

2.2 Theoretical results We shall not give here all the details allowing to determine closed-form expressions for the zero-field partition function, the spin-spin correlations, the static susceptibility as well as the correlation length. The reader may report himself to previous papers published by one of us [2, 3]. However we just give below the results obtained. In the thermodynamic limit ($N\rightarrow+\infty$) the zero-field partition function can be written as:

$$Z_N(0) = (4\pi)^{8N^2} \sum_{\ell=0}^{+\infty} \left[F_{\ell,\ell} \lambda_\ell(-\beta J_1) \lambda_\ell(-\beta J_2)\right]^{4N^2} , \tag{10}$$

where the factor $F_{\ell,\ell}$ is (the factor $1/4\pi$ being omitted):

$$F_{\ell,\ell} = (2\ell+1)^2 \sum_{L=0}^{2\ell} \frac{1}{2L+1} \left[C_{\ell\ 0\ \ell\ 0}^{L\ 0}\right]^4 , F_{0,0} = 1 . \tag{11}$$

In (11) the current L-coefficient is a Clebsch-Gordan (CG) one. The temperature-dependent function $\lambda_\ell(-\beta j)$ appearing in (10) is given by:

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

where $\mathrm{I}_{\ell+1/2}(-\beta j)$ is a modified Bessel function of the first kind.

As we are dealing with isotropic (Heisenberg) couplings, we have the following properties (with $v = x, y$ or z):

$$<S_{i,j}^v.S_{i+k,j+k'}^v> \ = \frac{1}{3} <\boldsymbol{S}_{i,j}.\boldsymbol{S}_{i+k,j+k'}> ,$$

$$<S_{i,j}^v> = \frac{1}{\sqrt{3}} <\boldsymbol{S}_{i,j}> , \ \Gamma_{i,j}^v = \frac{1}{3} \Gamma_{i,j} \ , \ <(S_{i,j}^v)^2> = \frac{1}{3} ,$$

$$\chi_{i,j}^v = \frac{\chi_{i,j}}{3} \ , \ \xi^v = \xi . \tag{13}$$

In addition we have found that $<S_{i,j}^z>$ =0, $<S_{i+k,j+k'}^z>$ =0, for T>0 K, so that the correlation function $\Gamma_{k,k'}^z$ reduces to the spin-spin correlation $<S_{i,j}^z.S_{i+k,j+k'}^z>$.

Of course, when $T = 0$ K exactly, we have $|<S^z_{i,j}>| = 1/3$ (or equivalently $|<\boldsymbol{S}_{i,j}>| = 1$). This result rigorously proves that the critical temperature is absolute zero, i.e., $T_C = 0$ K [3].

The spin-spin correlation in the thermodynamic limit ($N \to +\infty$) is given by [3]:

$$< S^z_{0,0}.S^z_{k,k'} >= \frac{1}{Z_N(0)}\sum_{\ell=0}^{+\infty} \left[F_{\ell,\ell}\lambda_\ell(-\beta J_1)\lambda_\ell(-\beta J_2)\right]^{4N^2}\left[X_{\ell+1}+(1-\delta_{\ell,0})X_{\ell-1}\right],\ k>0,\ k'>0,\ \text{as } N\to+\infty. \tag{14}$$

$Z_N(0)$ is the zero-field partition function given by (10), $\delta_{\ell,0}$ is the Dirac function and we have set:

$$X_{\ell+\varepsilon} = (C_{\ell+\varepsilon})^2 \frac{F_{\ell,\ell+\varepsilon}}{F_{\ell,\ell}}(u_{1,\ell+\varepsilon})^{k'}(u_{2,\ell+\varepsilon})^{k},\ k\ge 0,\ k'\ge 0,$$

$$C_{\ell+1} = \frac{\ell+1}{\sqrt{(2\ell+1)(2\ell+3)}},\ C_{\ell-1} = \frac{\ell}{\sqrt{(2\ell+1)(2\ell-1)}},\ u_{i,\ell+\varepsilon} = \frac{F_{\ell,\ell+\varepsilon}}{F_{\ell,\ell}}\frac{\lambda_{\ell+\varepsilon}(-\beta J_i)}{\lambda_\ell(-\beta J_i)},\ \varepsilon=\pm1,\ i=1,2. \tag{15}$$

$F_{\ell,\ell}$ is given by (11) and $F_{\ell,\ell+\varepsilon}$ can be expressed as the following CG-series (the factor $1/4\pi$ being omitted):

$$F_{\ell,\ell+\varepsilon} = (2\ell+1)(2\ell+2\varepsilon+1)\sum_{L=0}^{\min(2\ell,2\ell+2\varepsilon)} \frac{1}{2L+1}\left[C^{L\ 0}_{\ell\ 0\ \ell\ 0}C^{L\ 0}_{\ell+\varepsilon\ 0\ \ell+\varepsilon\ 0}\right]^2,\ F_{0,\varepsilon}=1,\ \varepsilon=\pm1. \tag{16}$$

The correlation length may be derived from (7) and (14)-(16):

$$\xi = \left[\frac{\sum_{\ell=0}^{+\infty}\left[F_{\ell,\ell}\lambda_\ell(-\beta J_1)\lambda_\ell(-\beta J_2)\right]^{4N^2}\left[N_{\ell+1}+(1-\delta_{\ell,0})N_{\ell-1}\right]}{\sum_{\ell=0}^{+\infty}\left[F_{\ell,\ell}\lambda_\ell(-\beta J_1)\lambda_\ell(-\beta J_2)\right]^{4N^2}\left[D_{\ell+1}+(1-\delta_{\ell,0})D_{\ell-1}\right]}\right]^{1/2},\ \text{as } N\to+\infty, \tag{17}$$

with:

$$D_{\ell+\varepsilon} = (C_{\ell+\varepsilon})^2\frac{F_{\ell,\ell+\varepsilon}}{F_{\ell,\ell}}\frac{1}{(1-|u_{1,\ell+\varepsilon}|)(1-|u_{2,\ell+\varepsilon}|)},\ N_{\ell+\varepsilon} = D_{\ell+\varepsilon}\left[\frac{|u_{1,\ell+\varepsilon}|(1+|u_{1,\ell+\varepsilon}|)}{(1-|u_{1,\ell+\varepsilon}|)^2}+\frac{|u_{2,\ell+\varepsilon}|(1+|u_{2,\ell+\varepsilon}|)}{(1-|u_{2,\ell+\varepsilon}|)^2}\right] \tag{18}$$

where $C_{\ell+\varepsilon}$, $u_{i,\ell+\varepsilon}$, $F_{\ell,\ell+\varepsilon}$ and $F_{\ell,\ell}$ are given by (15), (16) and (11), respectively.

The static susceptibility per unit cell and averaged per site may be written as:

$$\chi = \frac{1}{4}\left(\chi^z_{0,0}+\chi^z_{0,1}+\chi^z_{1,0}+\chi^z_{1,1}\right) \tag{19}$$

where the susceptibility per site is given by

$$\chi_{k,k'} = \frac{1}{Z_N(0)}\sum_{\ell=0}^{+\infty}\left[F_{\ell,\ell}\lambda_\ell(-\beta J_1)\lambda_\ell(-\beta J_2)\right]^{4N^2}\left[\chi_{\ell+1}+(1-\delta_{\ell,0})\chi_{\ell-1}\right],\ \text{as } N\to+\infty, \tag{20}$$

with $k = 0$ or 1 and $k' = 0$ or 1 so that owing to (19):

$$\chi_{\ell+\varepsilon} = \frac{\beta}{6}(C_{\ell+\varepsilon})^2\frac{F_{\ell,\ell+\varepsilon}}{F_{\ell,\ell}}\frac{(G^2+G'^2)W_{1,\ell+\varepsilon}+2GG'W_{2,\ell+\varepsilon}}{W_{3,\ell+\varepsilon}},\ \varepsilon=\pm1, \tag{21}$$

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

$$W_{3,\ell+\varepsilon} = [1-(u_{1,\ell+\varepsilon})^2][1-(u_{2,\ell+\varepsilon})^2], \tag{22}$$

where $C_{\ell+\varepsilon}$, $u_{i,\ell+\varepsilon}$, $F_{\ell,\ell+\varepsilon}$ and $F_{\ell,\ell}$ are given by (15), (16) and (11), respectively, as noted after (18).

3 Study of the low-temperature behaviors We have seen that the quantity $u_{i,\ell\pm1}$ given by (15) is of fundamental importance because it appears in the closed-form expression of the spin-spin correlation. The latter is involved in the respective definitions of the susceptibility and the correlation length ((6), (7)). Due to the fact that the critical temperature is absolute zero all the $\lambda_\ell(-\beta j)$ given by (12) (in fact the eigenvalues of the problem) become equivalent including that one characterized by infinite-ℓ. We have previously shown that the ratio $F_{\ell,\ell+\varepsilon}/F_{\ell,\ell}$ ($\varepsilon=\pm1$) tends to unity when $\ell\to+\infty$ [4]. As a result the low-temperature study of the ratio $u_{i,\ell\pm1}$ is reduced to that of $\lambda_{\ell\pm1}(-\beta J_i)/\lambda_\ell(-\beta J_i)$ or equivalently $I_{\ell\pm1+1/2}(-\beta J_i)/I_{\ell+1/2}(-\beta J_i)$ as $\ell\to+\infty$ and $\beta|J_i|\to+\infty$ (i=1,2). The behavior of Bessel function $I_{\ell+1/2}(-\beta|J_i|)\sim I_\ell(-\beta|J_i|)$ for $\ell\to+\infty$ and $\beta|J_i|\to+\infty$ has been established by Olver [5]. We have extended this work for a large-order ℓ (but not necessarily infinite) and for any real argument z_i varying from a finite value to infinity [4]. We have shown that it is necessary to introduce the dimensionless auxiliary variables:

$$\zeta_i=-\frac{J_i}{|J_i|}\left[\sqrt{1+z_i^{\,2}}+\ln\left(\frac{|z_i|}{1+\sqrt{1+z_i^{\,2}}}\right)\right],\ |z_i|=\frac{\beta|J_i|}{\ell}. \quad (23)$$

The numerical study of $|\zeta|$ is reported in Fig. 1. As expected we observe that there are two branches. $|\zeta|$ vanishes for a numerical value of $|z|^{-1}=\ell k_BT/|J|$ very close to $\pi/2$ so that there are 3 domains which will be physically interpreted below. Let T_0 be the corresponding temperature; we set:

$$\ell\frac{k_BT_0}{|J_i|}=\frac{\pi}{2},\ i=1,2. \quad (24)$$

In the formalism of renormalization group T_0 is called a fixed point. In the present 2*d* case we have $\ell\to+\infty$. As a result we derive that $T_0\to T_C$=0 K as $\ell\to+\infty$ so that the critical temperature may be seen as a fixed point. This will allow one to expand all the thermodynamic functions as Taylor series of current term $|T-T_0|$ near $T_0\approx T_C$=0 K.

At this step we must recall that the square of the spin modulus $S(S+1)\sim S^2$, as $S\to+\infty$, is absorbed in the exchange energy Chakravarty *et al.* [1] as well as Chubukov *et al.* [1] have written the action $S/\hbar$ (which allows one to calculate the partition function) as proportional to $J/2$. In addition these authors have considered the spin density S/a where a is the lattice spacing. In our case the lattice spacing between two similar Landé factors G or G' is $2a$. As a result, the left member of (24) can be written as $\ell k_BT_0/(|J|/2)(S/2a)^2$ so that the right-hand side becomes 4π instead of $\pi/2$. We must keep in mind this remark because it will be very useful later.

Under these conditions and after a tedious calculus the key ratio $u_{i,\ell\pm1}$ may be written as:

$$u_{i,\ell\pm1}(\ell|z_i|)=-\frac{J_i}{|J_i|}\left\{\mp\left(\frac{1}{|z_i|}+\frac{1}{2\ell|z_i|}\right)+\frac{1}{\theta_i|z_i|}\left[1-\frac{\theta_i}{2\ell}\right.\right.$$
$$\left.\left.-2\left(1-\frac{\theta_i}{4\ell}\right)\exp(-2\ell|\zeta_i|)+\ldots\right]\right\},\ i=1,2, \quad (25)$$

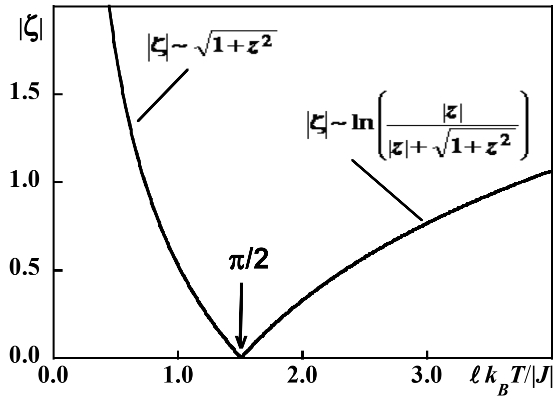

Figure 1 Variations of $|\zeta|$ for various values of $\ell k_BT/|J|$.

The previous general low-temperature expansion may be finally expanded as Taylor series near T_C=0 K if expressing the dimensionless auxiliary variables $|\zeta|$ and $|z|$ in this limit.

Noting that

$$\|z_i|-z_0|=\frac{1}{\ell}\frac{X_i}{T},\ X_i=\frac{|J_i|}{k_B}\frac{|T-T_0|}{T_0},\ X_i=\begin{cases}\rho_i, & T<T_0\\ \Delta_i, & T>T_0\end{cases}, \quad (26)$$

the Taylor series giving $|\zeta_i|$ becomes

$$|\zeta_i|=\ln\left(1+\frac{\pi}{2\ell}\frac{X_i}{T}\right),\ i=1,2, \quad (27)$$

so that:

$$\exp(-2\ell|\zeta_i|)=\left(1+\frac{\pi}{2\ell}\frac{X_i}{T}\right)^{-2\ell},\ i=1,2. \quad (28)$$

Noting that $(1\pm u/\ell)^\ell=\exp(\pm u)$, as ℓ large (or infinite), we finally derive:

$$\exp(-2\ell|\zeta_i|)=\exp\left(-\pi\frac{X_i}{T}\right),\ i=1,2,\text{ as }\ell\to+\infty. \quad (29)$$

The physical meaning of ρ_i and Δ_i will be given below.

At this step we define the coupling constants at temperature T and at the fixed point T_0:

$$g=\frac{k_BT}{|J|},\ g_0=\frac{k_BT_0}{|J|},\ \bar{g}=\frac{T}{T_0}. \quad (30)$$

These ratios measure the strength of the quantum fluctuations because, if we recall that $|J|$ must be read as $|J|S^2$, fluctuations are inversely proportional to S^2. If expanding

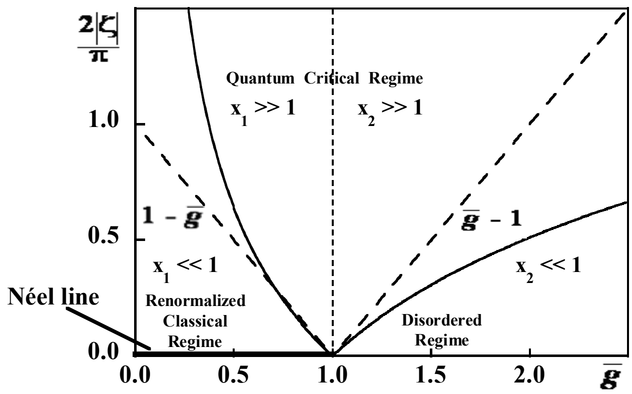

Figure 2 Diagram of magnetic phases near $T_0 = T_C = 0$ K.

$|\zeta|$ near T_0 we have the following equations:

$$|\zeta_F|_< = \frac{\pi}{2}(1-\bar{g}),\ (T < T_0),\ |\zeta_F|_> = \frac{\pi}{2}(\bar{g}-1),\ (T > T_0), \quad (31)$$

so that the thermal study of $|\zeta|$ is reduced to two domains $\bar{g} < 1$ i.e., $g < g_0$ ($T<T_0$) and $\bar{g} > 1$ i.e., $g > g_0$ ($T>T_0$). Each of these domains may be itself divided in two subdomains according to as $|\zeta|>|\zeta_F|$ or $|\zeta|<|\zeta_F|$. This is the reason for which we are led to introduce the $|\zeta_F|$-variables $x_1^i = T/|\zeta_F|_<$ and $x_2^i = T/|\zeta_F|_>$. Then using the variables ρ_i and Δ_i defined in (26) we set

$$x_1^i = \frac{2T}{\pi\rho_i},\ x_2^i = \frac{2T}{\pi\Delta_i}. \quad (32)$$

Thus, as noted by Chubukov *et al.* [1], the parameters x_1^i and x_2^i control the scaling properties of the magnetic system. ρ_i represents the spin stiffness of the ordered ground state (Néel state for an antiferromagnet) and Δ_i is a spin gap between the ground state and a spin liquid phase. ρ_i and Δ_i (*cf* (26)) vanish at the fixed point T_0. If we report to the definition of $|\zeta|$ (*cf.* (23)) $|\zeta|$ is dimensionless and homogeneous to T_0/T i.e., $1/\bar{g}$. If $\bar{g} < 1$ ($T<T_0$) we have two possibilities $x_1^i > 1$ i.e., $T>|\zeta_F|_<$ and $x_1^i < 1$ i.e., $T<|\zeta_F|_<$. When $T=T_0$, x_1^i and x_2^i become infinite due to the fact that ρ_i and Δ_i vanish. Finally, if $\bar{g} > 1$ ($T>T_0$) we have two possibilities $x_2^i > 1$ i.e., $T>|\zeta_F|_>$ and $x_2^i < 1$ i.e., $T< |\zeta_F|_>$. As there is an analytical continuity between x_1^i and x_2^i while passing through T_0, see (26), we derive that there are 3 domains: (i) if $T<|\zeta_F|_<$ ($x_1^i < 1$) we deal with the *Renormalized Classical Regime* (RCR), (ii) if $T<|\zeta_F|_>$ ($x_2^i < 1$) we deal with the *Quantum Disordered Regime* (QDR) and (iii) if $T>|\zeta_F|_<$ ($x_1^i > 1$) or $T>|\zeta_F|_>$ ($x_2^i > 1$) we have the *Quantum Critical Regime* (QCR). Along the line $T=T_0$ in this domain we directly reach the fixed point without a phase change. The magnetic diagram has been reported in Fig. 2. It is strictly similar to the one obtained by Chakravarty *et al.* and Chubukov *et al.* [1], separately. Finally, if T tends towards absolute zero when coming from the Renormalized Classical Regime (RCR) or from the Quantum Disordered Regime (QDR), or directly tends to the fixed point T_0 when coming from the Quantum Critical Regime (QCR), we directly reach the Néel line.

As noted before (25) we use the conventional notation of Chakravarty *et al.* and Chubukov *et al.* [1] for it allows one to make a reasoning with the simplest lattice unit cell of spacing a (instead of $2a$ in the more general case). Thus we reduce the physical discussion to the particular case $G=G'$. Consequently, instead of x_k^i , we now use $\tilde{x}_k^i = x_k^i/4$. As $\ell\,\big||z|-z_0\big| >> 1$ we deal with very low-temperature phases: the Renormalized Classical Regime (RCR, $\tilde{x}_1^i$ <<1) and the Quantum Disordered Regime (QDR, $\tilde{x}_2^i$ <<1). Using the relation between $\tilde{x}_1^i$ and ρ_i on the one hand, and between $\tilde{x}_2^i$ and Δ_i on the other hand, we have $\rho_i>>T$ and $\Delta_i>>T$, respectively. Expanding $u_{i,\ell\pm1}$ in the variable $\tilde{x}_k^i$ we obtain after complicated calculations:

$$u_{i,\ell\pm1}(\ell|z_i|) \mp \frac{J_i}{|J_i|}\left(\frac{1}{|z_i|}+\frac{1}{2\ell|z_i|}\right) = -\frac{J_i}{|J_i|}\Big\{ 1-\Big[2\tilde{x}_k^i + \frac{8\pi}{e}\left(1-\tilde{x}_k^i\right).\exp\left(-1/2\tilde{x}_k^i\right)\Big]+...\Big\},\ \tilde{x}_k^i < 1,\ k = 1, 2. \quad (33)$$

For both regimes $\tilde{x}_1^i$ <<1 and $\tilde{x}_2^i$ <<1 a short numerical study shows that the exponentiel term is dominating over the term 2 $\tilde{x}_k^i$ so that:

$$u_{i,\ell\pm1}(\ell|z_i|) \mp \frac{J_i}{|J_i|}\left(\frac{1}{|z_i|}+\frac{1}{2\ell|z_i|}\right) = -\frac{J_i}{|J_i|}\Big\{ 1 - \frac{8\pi}{e}\left(1-\tilde{x}_k^i\right).\exp\left(-1/2\tilde{x}_k^i\right)+...\Big\},\ i = 1, 2,\ k = 1, 2. \quad (34)$$

In the Quantum Critical Regime (QCR, x_1^i >1 and x_2^i >1), we now have $\ell\,\big||z|-z_0\big| << 1$. As a result, due to (26) and (32), the expansion must be in $1/(4\pi\,\tilde{x}_k^i)$. We have

$$u_{i,\ell\pm1}(\ell|z_i|) \mp \frac{J_i}{|J_i|}\left(\frac{1}{|z_i|}+\frac{1}{2\ell|z_i|}\right) = -\frac{J_i}{|J_i|}\frac{\pi}{2}\Big\{ 1 + \frac{2}{\pi}\left(\frac{1}{4\pi\tilde{x}_k^i}\right) - 2\left(\frac{1}{4\pi\tilde{x}_k^i}\right)^2 + ...\Big\}\ i = 1, 2,\ k = 1, 2. \quad (35)$$

Using again the relation between $\tilde{x}_1^i$ and ρ_i on the one hand, $\tilde{x}_2^i$ and Δ_i on the other hand, we now have $\rho_i<<T$ and $\Delta_i<<1$, respectively.

Reporting these various expressions in the definitions of the correlation length and the susceptibility respectively given by (7) and (6) we can write:

$$\frac{\xi}{2a} \approx \beta|J|,\ \text{Néel line}\ \tilde{x}_1 << 1,\ \text{(QCR)}\ \tilde{x}_1 > 1, \quad (36a)$$

$$\frac{\xi}{2a} \approx \frac{e}{8\pi}\frac{\sqrt{2}}{2}\left(1+\frac{T}{4\pi\rho^{\mathrm{Ch}}}\right)\exp\left(\frac{2\pi\rho^{\mathrm{Ch}}}{T}\right),$$

$$\text{(RCR)}\ \tilde{x}_1 < 1. \quad (36b)$$

where ρ^{Ch} represents the spin stiffness of the model proposed by Chakravarty *et al.* and Chubukov *et al.* [1]. The correspondence with our model is $\rho=2\rho^{Ch}$ (i.e., $J=2J^{Ch}$). It is well-know that, near $T_C=0$ K, the product χT behaves as $\xi_x\xi_y\mathcal{M}^2$ where $\mathcal{M}$ is the magnetic moment per unit cell. In our case, as we restrict our study to $J=J_1=J_2$, we have $\xi=\xi_x=\xi_y$ where the correlation length is given by (36). Thus, for 2*d* non-compensated moments i.e., for ferromagnetic (F) or antiferromagnetic (AF) couplings, χT diverges as ξ^2:

$$\chi T \approx (\beta|J|)^2, \text{ Néel line } \tilde{x}_1 << 1, \text{ (QCR) } \tilde{x}_1 > 1, \mathcal{M}(T) \neq 0,$$
$$J > 0 \text{ (AF couplings)}, J < 0 \text{ (F couplings)}, \quad (37a)$$

$$\chi T \approx \exp\left(\frac{4\pi\rho^{Ch}}{T}\right), \text{ (RCR) } \tilde{x}_1 < 1, \mathcal{M}(T) \neq 0,$$
$$J > 0 \text{ (AF couplings)}, J < 0 \text{ (F couplings)}. \quad (37b)$$

In the compensated case the product χT may be written as:

$$\chi T \approx \frac{G^2}{3}\left(\frac{k_B T}{2J}\right)^2, \mathcal{M}(T) \to 0, \text{ as } T \to 0 \text{ K}$$
$$J > 0 \text{ (AF couplings)}. \quad (38)$$

These results are in perfect agreement with the corresponding ones obtained by the renormalization group method [1].

In order to give an illustration of the theoretical model developed in this paper we have fitted the experimental susceptibility measured for a powder sample concerning the compound $[\{Mn(DENA)_2(N_3)_2\}_n]$ because the corresponding Néel temperature T_N=2.0 K is very low (the ligand DENA stands for the group diethylnicotinamide). This compound is characterized by 2*d* square lattices of classical spins (the manganese ions) isotropically coupled (i.e., showing Heisenberg couplings). That means that the 2*d* magnetic behavior occurs in the low-temperature region. The corresponding fit of the product χT is reported Fig. 3. $[\{Mn(DENA)_2(N_3)_2\}_n]$ is characterized by antiferromagnetic couplings (i.e., compensated magnetic moments). The experimental Landé factor G=1.98 $\mu_B/\hbar$ is very close to the theoretical value 2. Similarly, the exchange energy J/k_B=4.15 K is in agreement with tabulated experimental values previously obtained.

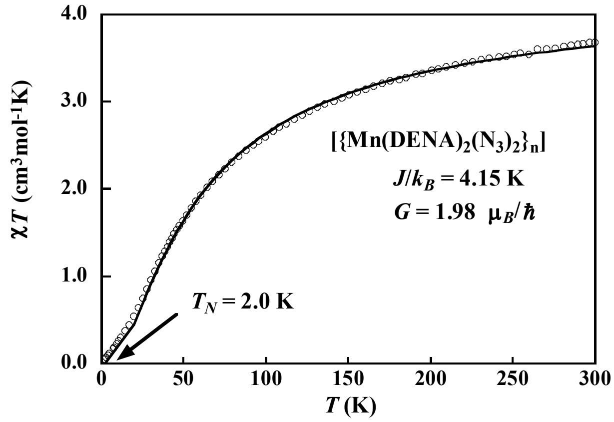

Figure 3 Theoretical fit of the experimental susceptibility for $[\{Mn(DENA)_2(N_3)_2\}_n]$ (the ligand DENA stands for the group diethylnicotinamide).

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