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Analytical Solution of the $2d$ Classical Heisenberg Model.

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Abstract. – For the first time we exactly establish the term of higher degree in the polynomial expansion of the zero-field partition function. In the infinite-layer limit, we derive analytical expressions for the spin-spin correlations, the susceptibility and the specific heat, and we examine their respective behaviours near the critical temperature $T_c = 0$ K. We calculate the analytical values of critical exponents α, γ, η and ν.

In this article we rigorously examine the case of classical spins belonging to a two-dimensional square lattice and characterized by Heisenberg couplings between nearest neighbours. So far, approximate techniques have been used for studying this problem: high-temperature series expansions [1], spin-wave theory [2], Green's function approaches [3], renormalization group [4], Monte Carlo simulations [5], decomposition of the planar lattice into interacting linear chains [6]. A general survey of the thermodynamics and experimental behaviour of two-dimensional magnets has been reported by de Jongh [7]. Recent theoretical developments [8] as well as experimental ones [9] have motivated the present work. In a famous paper Mermin and Wagner have shown that no long-range order is stable at any non-zero temperature for one- and two-dimensional structures [10]. In this work we rigorously point out that the transition temperature is 0 K so that the 2D isotropically coupled classical spin systems have a quasi-infinite critical domain. In addition we exactly calculate the critical exponents α, γ, η and ν.

Let us consider a square lattice of $(2N+1)^2$ sites (i, j); each host site is described by a classical spin moment and is characterized by a Heisenberg exchange coupling between nearest neighbours; in addition each moment is submitted to an external magnetic field B applied along the z-axis of quantization. The corresponding Hamiltonian may be written

$$H = \sum_{i=-N}^{N-1} \sum_{j=-N}^{N-1} H_{i,j}^{\mathrm{ex}} + \sum_{i=-N}^{N} \sum_{j=-N}^{N} H_{i,j}^{\mathrm{mag}} \tag{1}$$

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with

$$H^{\text{ex}}_{i,j} = (J_1 S_{i,j+1} + J_2 S_{i+1,j}) S_{i,j}\,, \qquad H^{\text{mag}}_{i,j} = -G_{i,j} S^z_{i,j} B\,. \tag{2}$$

In this writing, $J_i > 0$ (with $i = 1, 2$) denotes an antiferromagnetic coupling. $G_{i,j}$ is Landé's factor associated to the classical spin moment ($G_{i,j} = G$, for $i+j$ even, $G_{i,j} = G'$, for $i+j$ odd). The zero-field partition function $Z_N(0)$ is obtained by integrating the operator $\exp[-\beta H^{\text{ex}}]$ over all the angular variables characterizing the states of all the classical spins belonging to the lattice (β is Boltzmann's factor and will not have to be confused with the critical exponent β_c). Because of the classical character of these moments, all the operators $H^{\text{ex}}_{i,j}$ commute so that it is possible to separate all the contributions corresponding to each site (i, j). Therefore the operator $\exp[-\beta H^{\text{ex}}]$ appears as the product over i and j of operators $\exp[-\beta H^{\text{ex}}_{i,j}]$; we then have to expand these operators (characterized by an argument involving a product such as $S_{k,k'} S_{i,j}$, with $(k, k') = (i, j+1)$ or $(i+1, j)$) on the infinite basis of spherical harmonics. Thus the zero-field partition function may be written:

$$Z_N(0) = (4\pi)^{4N(2N+1)} \sum_{l_{N,-N}=0}^{+\infty} \lambda_{l_{N,-N}}(-\beta J_1) \sum_{l'_{N,-N}=0}^{+\infty} \lambda_{l'_{N,-N}}(-\beta J_2) \ldots \cdot$$

$$\cdot \sum_{l_{-N,N}=0}^{+\infty} \lambda_{l_{-N,N}}(-\beta J_1) \sum_{m_{N,-N}=-l_{N,-N}}^{+l_{N,-N}} \; \sum_{m'_{N,-N}=-l'_{N,-N}}^{+l'_{N,-N}} \cdots \sum_{m_{-N,N}=-l_{-N,N}}^{+l_{-N,N}} \cdot$$

$$\cdot \prod_{k_1=-N}^{N} \prod_{k_2=-N}^{N} \int \mathrm{d}S_{k_1,k_2} Y_{l'_{k_1+1,k_2}, m'_{k_1+1,k_2}}(S_{k_1,k_2}) Y_{l_{k_1,k_2-1}, m_{k_1,k_2-1}}(S_{k_1,k_2}) \cdot$$

$$\cdot Y^*_{l_{k_1,k_2}, m_{k_1,k_2}}(S_{k_1,k_2}) Y^*_{l'_{k_1,k_2}, m'_{k_1,k_2}}(S_{k_1,k_2})\,, \tag{3}$$

where $\lambda_l(-\beta J_1)$ is the modified Bessel function of the first kind $I_{l+1/2}(-\beta J_1)$ multiplyed by the factor $(\pi/2\beta J_i)^{1/2}$. Note that, in eq. (3), when the current site (i, j) belongs to an edge (respectively, to a corner) of the lattice, the current integral is reduced to a product of three (respectively, two) spherical harmonics. Let $F_{i,j}$ be this current integral; it is readily shown that

$$F_{i,j} = (-1)^{m_{i,j}+m'_{i,j}} \sum_{L=L_<}^{L_>} \sum_{M=-L}^{+L} (-1)^M \left[\frac{(2l'_{i+1,j}+1)(2l_{i,j-1}+1)(2l_{i,j}+1)(2l'_{i,j}+1)}{(4\pi)^2 (2L+1)^2} \right]^{1/2} \cdot$$

$$\cdot C^{L0}_{l'_{i+1,j}0\, l_{i,j-1}0}\, C^{LM}_{l'_{i+1,j}-m'_{i+1,j} l_{i,j-1}-m_{i,j-1}}\, C^{L0}_{l_{i,j}0\, l'_{i,j}0}\, C^{L\,-M}_{l_{i,j}m_{i,j} l'_{i,j}m'_{i,j}}\,, \tag{4}$$

where $L_<$ and $L_>$ will be specified below. $C^{l_3 m_3}_{l_1 m_1 l_2 m_2}$ is a Clebsch-Gordan coefficient (for an integral involving three spherical harmonics the L-summation disappears and $F_{i,j}$ reduces to a product of two coefficients; the two other coefficients reduce to unity because the non-existing bonds of the lattice are characterized by vanishing values of l's and m's). The non-vanishing condition of the Clebsch-Gordan coefficients gives triangular inequalities; in other words L must belong to the ranges $[|l'_{i+1,j} - l_{i,j-1}|, l'_{i+1,j} + l_{i,j-1}]$ and $[|l_{i,j} - l'_{i,j}|, l_{i,j} + l'_{i,j}]$, respectively: Thus $L_<$ must be equal to $\max(|l'_{i+1,j} - l_{i,j-1}|, |l_{i,j} - l'_{i,j}|)$ and $L_>$ must be $\min(l'_{i+1,j} + l_{i,j-1}, l_{i,j} + l'_{i,j})$. By using the symmetry properties of these coefficients with respect to the various permutations over L and the involved l's and l''s so that $F_{i,j}$ is unchanged, it is possible to obtain two other couples of triangular inequalities which must be compatible simultaneously. Therefore, as all the integrals are imbricated, one has to determine the solution $(\ldots, l_{i,j}, \ldots, l'_{i,j}, \ldots)$ for the whole lattice by taking into account all the triangular inequalities. Of course there exist a great number of solutions but a single one allows to obtain the term of higher degree in the λ_l-polynomial expansion of $Z_N(0)$: This occurs when all the $l_{i,j}$'s and all the $l'_{i,j}$'s are equal to a common positive (or null) value l. Then, as the coefficient $C^{L0}_{l'_{i+1,j}0\, l_{i,j-1}0}$ ($C^{L0}_{l_{i,j}0\, l'_{i,j}0}$, respectively) does not vanish if $l'_{i+1,j} + l_{i,j-1} + L$ ($l_{i,j} + l'_{i,j} + L$, respectively) is equal to an even positive number (or zero), note that L must be even (or equal to zero). Thus all the imbricated l-summations involved in eq. (3) reduce to a single one. For obtaining the other terms of lower degree in the polynomial expansion of $Z_N(0)$, a numerical work is unavoidable when the number of lattice sites is finite. However, one can note that all the l-series rapidly converge for small values of l because, for a same argument and whatever its numerical value, the functions $\lambda_l(-\beta J_i)$ (which are modified Bessel functions of the first kind $I_{l+1/2}(-\beta J_i)$) rapidly decrease when l increases: Therefore the numerical work can be rapidly achieved.

Another non-vanishing condition of the Clebsch-Gordan coefficients $C^{LM}_{l'_{i+1,j}-m'_{i+1,j}l_{i,j-1}-m_{i,j-1}}$ and $C^{L-M}_{l_{i,j}m_{i,j}l'_{i,j}m'_{i,j}}$ concerns the relative integers $m_{i,j}$'s and $m'_{i,j}$'s. As the current value M must be equal to $-(m'_{i+1,j} + m_{i,j-1})$ and to $-(m'_{i,j} + m_{i,j})$ simultaneously it is equivalent to say that the sum $m_{i,j-1} + m'_{i+1,j} - m_{i,j} - m'_{i,j}$ vanishes. Among all the solutions $(\ldots, m_{i,j}, \ldots, m'_{i,j}, \ldots)$, we always have the trivial one $m_{i,j} = 0$, $m'_{i,j} = 0$. But in the general case the numerical determination of coefficients $m_{i,j}$ and $m'_{i,j}$ is unavoidable. However we have pointed out the following algorithm:

$$m_{i,j} = \sum_{k=j+1}^{N} (m'_{i,k} - m'_{i+1,k}), \quad \forall(i,j), \qquad m'_{i,-N} = -\sum_{k=-(N-1)}^{N} m'_{i,k}, \quad \forall i, \tag{5}$$

the other coefficients $m'_{i,j}$ (with $j \geq -(N-1)$) being undetermined (*i.e.* there remains $4N^2$ unknowns instead of the initial $4N(2N+1)$ ones). Moreover the sum of all the $m'_{i,j}$'s (all the $m_{i,j}$'s, respectively) belonging to a same line i of the lattice (a same row j, respectively) vanishes (this can be easily derived by adding all the vanishing sums $m_{i,j-1} + m'_{i+1,j} - m_{i,j} - m'_{i,j}$ obtained for all the sites (i,j)). After assuming this numerical work the zero-field partition function can be completely determined. Thus the λ_l-polynomial expansion of $Z_N(0)$ may be written:

$$Z_N(0) = \sum_{l=0}^{+\infty} [(4\pi)^2 \lambda_l(-\beta J_1)\lambda_l(-\beta J_2)]^{2N(2N+1)} \sum_{m_{N,-N}=-l}^{+l} \sum_{m'_{N,-N}=-l}^{+l} \cdots \sum_{m_{-N,N}=-l}^{+l} \cdot \prod_{k_1=-N}^{+N} \prod_{k_2=-N}^{+N} F_{k_1,k_2} + \ldots \tag{6}$$

Note that, in the above formula, the dots recall that there exist other terms of lower degree in the λ_l-polynomial expansion. In the infinite-lattice limit, $Z_N(0)$ reduces to the higher term, *i.e.* $[(4\pi)^2 \lambda_0(-\beta J_1)\lambda_0(-\beta J_2)]^{2N(2N+1)}$.

Then the specific heat per site (i,j) labelled C can be easily derived:

$$C = k_B \sum_{i=1}^{2} (\beta J_1)^2 \left[\frac{\lambda_2(-\beta J_i)}{\lambda_0(-\beta J_i)} - \left(\frac{\lambda_1(-\beta J_i)}{\lambda_0(-\beta J_i)} \right)^2 \right]. \tag{7}$$

But the most interesting quantity is the susceptibility per site (i,j) labelled $\chi_{i,j}$: It can be evaluated by assuming the various summations over k and k' (between $-N$ and $+N$) of the current term $\beta G_{i,j} G_{i+k,j+k'} \langle S^z_{i,j} S^z_{i+k,j+k'} \rangle$ (note that, because of the presence of isotropic couplings, the three susceptibilities $\chi^{xx}_{i,j}$, $\chi^{yy}_{i,j}$ and $\chi^{zz}_{i,j}$ are equal so that $\chi_{i,j}$ globally represents the susceptibility labelled χ). Thus the calculation of χ reduces to that of spin-spin correlations. Each correlation $\langle S^z_{i,j} S^z_{i+k,j+k'} \rangle$ can be defined by a fraction the denominator of which is $Z_N(0)$. The expression of the numerator can be given by that of $Z_N(0)$ (cf. eq. (3)) but now one must introduce the extra terms $\cos\theta_{k_1,k_2}$ at sites $(k_1, k_2) = (i, j)$ and $(k_1, k_2) = (i + k, j + k')$. By using the decomposition law of the current term $\cos\theta_{k_1,k_2} Y_{l_{k_1,k_2}, m_{k_1,k_2}}(S_{k_1,k_2})$ *vs.* $Y_{l_{k_1,k_2}+1, m_{k_1,k_2}}(S_{k_1,k_2})$ and $Y_{l_{k_1,k_2}-1, m_{k_1,k_2}}(S_{k_1,k_2})$, respectively, the calculation of this numerator is similar to that one encountered for evaluating $Z_N(0)$. In the particular case of the infinite lattice, one can say that the term of higher degree of the numerator will be obtained for $l_{ij} = l'_{ij} = 0$ for all the sites which are outside a rectangle defined between sites (i, j), $(i + k, j)$, $(i, j + k')$ and $(i + k, j + k')$—note that, in the present case, the decomposition law is reduced to the single term $Y_{1,0}(S)$. For each site belonging to the rectangle there are two possibilities for choosing $l_{i,j}$ and $l'_{i,j}$ ($l_{i,j} = 1$, $l'_{i,j} = 0$ or $l_{i,j} = 0$, $l'_{i,j} = 1$) which lead to a non-vanishing contribution. In other words there exits several paths of integration between sites (i, j) and $(i + k, j + k')$ but globally they lead to the same result. Finally we have

$$\langle S^z_{i,j} S^z_{i+k,j+k'} \rangle \sim \frac{1}{3}\left(\frac{\lambda_1(-\beta J_1)}{\lambda_0(-\beta J_1)}\right)^{|k|}\left(\frac{\lambda_1(-\beta J_2)}{\lambda_0(-\beta J_2)}\right)^{|k'|}, \quad \text{as } N \to +\infty . \tag{8}$$

It must be noted that each of the preceding ratios is nothing more than Langevin's function $\mathscr{L}(-\beta J_1)$. Then the susceptibility χ can be evaluated (due to the alternating character of the distribution of Landé factors the susceptibility per unit cell automatically contains the four contributions χ_{00}, χ_{01}, χ_{10} and χ_{11}). Noting that, because of the separate contributions of lines i and rows j which appear in the expression of the spin-spin correlations, on the one hand, and the fact that each ratio $\lambda_1(-\beta J_1)/\lambda_0(-\beta J_i)$ is always lower than unity (in absolute value), on the other hand, the two summations over k and k' are easily achieved by exclusively taking into account the relevant correlations; we then have

$$\chi = \frac{\beta}{6}\,\frac{(G^2 + G'^2)W_1 + 2GG'W_2}{(1 - u_1^2)(1 - u_2^2)} \quad \text{as } N \to +\infty , \tag{9}$$

with

$$W_1 = (1 + u_1^2)(1 + u_2^2) + 4u_1u_2, \qquad W_2 = 2u_1(1 + u_2^2) + 2u_2(1 + u_1^2), \tag{10}$$

where u_1 and u_2 are $\mathscr{L}(-\beta J_1)$ and $\mathscr{L}(-\beta J_2)$, respectively. Note that, if $u_1 = 0$ or $u_2 = 0$ (*i.e.* $J_1 = 0$ or $J_2 = 0$), one finds again Fisher's result concerning the susceptibility of a classical spin chain [11].

The correlation length ξ can be defined by the mean quadratic distance $k^2 + k'^2$ between the origin site $(0, 0)$ and site (k, k') weighted by the corresponding correlation $|\langle S^z_{0,0} S^z_{k,k'}\rangle|$; similarly correlation lengths ξ_1 and ξ_2 can be defined for the lines of the lattice characterized by the exchange energies J_1 and J_2, respectively. Thus ξ appears to be equal to $((\xi_1)^2 + (\xi_2)^2)^{1/2}$, where ξ_i globally behaves as $(1 - u_i^2)^{-1}$ (with $i = 1, 2$). When the critical temperature is reached ξ_1 and ξ_2 diverge simultaneously: It occurs when $|u_i|$ (*i.e* $|\mathscr{L}(-\beta J_i)|$) tends to unity. In other words this situation will intervene when temperature tends to 0 K [12]. Consequently 2D lattices composed of classical spins isotropically coupled are characterized by a quasi-infinite critical domain: The short-range order remains important whereas the long-range one is absent, except at 0 K where it becomes preponderant. ξ behaves as $\beta((J_1)^2 + (J_2)^2)^{1/2}$: Thus the corresponding critical exponent ν is such that $\nu = 1$. In the zero-temperature limit and for non-compensated spin sublattices ($G \neq G'$), the susceptibility χ diverges according to a β^3-law; subsequently the associated critical exponent is: $\gamma = 3$. This theoretical result has the same value as that obtained by Fisher by using the renormalization group approach [13] and improves the first estimate of Stanley and

Kaplan [14] obtained with high-temperature series expansions ($\gamma = 2.75 \pm 0.05$). In addition χ appears as the vanishing limit of the q-dependent correlation function $g(q)$ (which is the Fourier transform of χ); near the critical temperature $T_c = 0$ K $g(0)$ (*i.e.* χ) behaves as $\beta^{2-\eta}$ what permits us to derive the critical exponent $\eta = -1$. Consequently Fisher's scaling law ($\gamma = \nu(2-\eta)$) is fulfilled. At this step it must be noted that, in the low-temperature range (*i.e.* near the critical temperature), the spin-spin correlation $|\langle S^z_{0,0} S^z_{k,k'}\rangle|$ given by eq. (8) behaves as $1 - |k|/\beta|J_1| - |k'|/\beta|J_2|$ *i.e.* as $1 - |k|/\xi_1 - |k'|/\xi_2$ (in absolute value). In other words the decay of critical correlation (which is described by the general power law $r^{-(D-2+\eta)}$ is characterized by the critical exponent $\eta = 1$ but this does not naively mean that this correlation increases with the distance.

In fact the interpretation of the low-temperature behaviour of χ is more subtle. It is easily shown that the product χT behaves as $\xi_1 \xi_2 \mathscr{M}^2$, where $\mathscr{M}$ is the temperature-dependent magnitude of the magnetic moment per unit cell ($\mathscr{M}$ also depends on the sign of the exchange energies J_1 and J_2). Thus, in the low-temperature range, the lattice can be considered as an assembly of quasi-independent quasi-rigid rectangular blocks of lengths ξ_1 and ξ_2, respectively, where ξ_1 and ξ_2 are the correlation lengths defined above. For non-compensated sublattices ($G \neq G'$, $J_1 < 0$, $J_2 < 0$ or $J_1 > 0$, $J_2 > 0$) χT diverges as ξ_1, ξ_2, *i.e.* according to a β^2-law; for compensated sublattices ($G = G'$, $J_1 > 0$, $J_2 > 0$) the behaviour of χT appears as a competition between the divergence of the product of correlation lengths ξ_1 and ξ_2 and the evanescence of $\mathscr{M}$, the magnetic moment per unit cell. It has been previously shown that $\mathscr{M}$ vanishes according to a T-polynomial [15]: thus, if $G = G'$ and $J_1 > 0$, $J_2 > 0$, χT vanishes according to a T^2-law. Another possibility of compensation can occur if J_1 and J_2 have opposite signs whatever G and G'; in that case χT tends to a finite constant limit (which depends on J_1 and J_2) according to a T-law. At this step it must be noted that, for lattices characterized by different exchange energies J_1 and J_2, a change of regime appears when $k_B T/|J_2|$ is of the same order of magnitude as ξ_1, *i.e.* $k_B T_{CO} \sim \sqrt{|J_1 J_2|}$: Coming from high temperatures where the chain behaviour is dominant, this crossover phenomenon occurs when $k_B T$ reaches the value $\sqrt{|J_1 J_2|}$ and the planar behaviour becomes preponderant (if J_2 is chosen lower than J_1 this phenomenon can be clearly observed in the low-temperature range). As for the specific heat per site C, it tends to 2 when temperature tends to 0 K; the corresponding critical exponent is such as $\alpha = 0$. In that case too this theoretical result is in good agreement with that obtained by Jasnow and Wortis [16] by using high-temperature series expansions ($\alpha \approx 0.10 \pm 0.01$). Therefore, Josephson's scaling law $\alpha = 2 - \nu D$, where D is the layer dimensionality, is fulfilled.

As a final comment we can note that the method which has been used for calculating the beginning of the polynomial expansion of the zero-field partition function $Z_N(0)$ is nothing more than the transfer matrix one. In the present case the involved matrix has an infinite size and is applied to eigenfunctions represented by spherical harmonics; in addition the corresponding eigenvalues, for each current site, are given by the various λ_l's. Therefore it is not surprising that the term of higher degree in the polynomial expansion of $Z_N(0)$ given by eq. (6) contains the higher selected eigenvalues which appear in the trace of the final diagonal matrix after successive applications to the $(2N+1)^2$ sites of the lattice.

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