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Quasi-long-range ordering in a finite-size 2D classical Heisenberg model

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Received 24 November 2006, in final form 13 February 2007

Published 20 March 2007

Online at stacks.iop.org/JPhysA/40/3741

Abstract

We analyse the low-temperature behaviour of the classical isotropic ferromagnetic Heisenberg model on a two-dimensional square lattice of finite size. Presence of a residual magnetization in a finite-size system enables us to use a low-temperature approximation, which is however more restricting than the usual spin-wave approximation known to give reliable results for the XY model at low temperatures T . For the system considered, we find that the spin–spin correlation function decays as $1/r^{\eta(T)}$ for large separations r bringing about the presence of a quasi-long-range ordering. We give analytic estimates for the exponent $\eta(T)$ in different regimes and support our findings by Monte Carlo simulations of the model on lattices of different sizes at different temperatures.

PACS numbers: 05.50.+q, 75.10

The long history of the Heisenberg model in two dimensions (2D) is characterized by a competition between two contrary opinions about the properties of this model. The early observation, made by Peierls [1], about long-wavelength lattice waves destroying the localization of particles on their lattice sites in two-dimensional crystals was followed later by a similar result for 2D magnets of continuous symmetry where the spontaneous magnetization is destroyed by long-wavelength spin waves. Proven mathematically by Mermin and Wagner [2], this fact denied the very possibility of a ferromagnetic phase transition in this type of systems, although the high-temperature series for the Heisenberg and XY models in 2D, presented by Stanley and Kaplan [3] approximately at the same time, gave indication of a phase transition in both models. Being qualitatively similar in those works, the two models had quite different developments afterwards. The 2D XY model has become famous for the Berezinskii–Kosterlitz–Thouless (BKT) transition [4] to a quasi-long-range ordered (QLRO)

phase. This special type of ordering cannot be characterized by an order parameter in the infinite system and manifests in a power-law decay of the spin–spin correlation function with distance. The low-temperature properties and critical behaviour of the XY model on a 2D lattice are governed by interactions between topological defects which appear in the system [5–7]. This scenario is deeply connected to the symmetry of the model. In the XY model, rotations of a spin form an Abelian group that allows for the formation of stable topological defects such as spin vortices and others; in this sense it can be called an Abelian model in contrast to the non-Abelian ones. The Heisenberg model is non-Abelian; this is the main reason to deny a possibility of a BKT transition in it. The crucial evidence for an absence of a phase transition in the 2D Heisenberg model came from the renormalization treatment made by Polyakov [8, 9]. Now it is commonly believed that this model does not exhibit any phase transition at non-zero temperatures, although there are still some controversies (see e.g. [10–14]) and reports were made that disagree with the outcome of Polyakov’s work, assuming the possibility of a phase transition at finite temperature in the 2D Heisenberg model, similar to the BKT transition in the 2D XY model (see [7] and references therein). The last question is important in the context of an asymptotic freedom of QCD at 4D [9, 15].

The discussion above concerns *infinite systems*. It is an infinite 2D model of continuous symmetry for which the Mermin–Wagner theorem has been proven. However, either in Monte Carlo simulations or even in reality we always deal with finite physical systems. It is now well known that in a finite 2D XY spin system below the BKT transition temperature, there is a non-vanishing magnetization which tends to zero only in the thermodynamic limit [16, 17]. This observation goes back to Berezinskii himself and is supported by experimental measurements (see [18]).

Although there is still no definite answer for the question whether the 2D Heisenberg model can pass to a QLRO phase or not, it is reasonable to assume that this model considered on a finite lattice will certainly possess some ordering, i.e. non-vanishing magnetization, at low temperatures similar as the 2D XY model does. This assumption is clear from the obvious fact that in a finite system, transition to the ordered phase at $T = 0$ (when all spins of the Heisenberg model are pointed in the same direction) must be continuous. Hence, we must see an appearance of some ordering as the temperature approaches zero. This is confirmed by MC simulations on the Heisenberg model in two dimensions [19].

Due to the above reasonings, we assume all spins (vectors) $\mathbf{S}_{\mathbf{r}} = (S_{\mathbf{r}}^x, S_{\mathbf{r}}^y, S_{\mathbf{r}}^z)$ in the Hamiltonian of the classical Heisenberg model on a two-dimensional square lattice of size $N = L \times L$ with spacing a and sites defined by a vector \mathbf{r} :

$$H = -\frac{1}{2} \sum_{\mathbf{r}} \sum_{\mathbf{r}'} J(\mathbf{r} - \mathbf{r}') (S_{\mathbf{r}}^x S_{\mathbf{r}'}^x + S_{\mathbf{r}}^y S_{\mathbf{r}'}^y + S_{\mathbf{r}}^z S_{\mathbf{r}'}^z), \quad (1)$$

being pointed approximately in the same direction at low enough temperatures. This approximation, referred hereafter to as the low-temperature approximation, is more restricting than the usual spin-wave approximation (SWA) which assumes that the *differences* between neighbouring spin orientations are small. We consider the case of the nearest neighbours’ interaction potential $J(\mathbf{r} - \mathbf{r}') = J\delta_{|\mathbf{r}-\mathbf{r}'|,a}$, ($J > 0$), and $1/2$ stands in (1) to prevent the double count of each bond.

We choose a special system of the angle coordinates $\theta_{\mathbf{r}}^{(1)}, \theta_{\mathbf{r}}^{(2)}$ (see figure 1), defined by the relations

$$S_{\mathbf{r}}^x = \cos \theta_{\mathbf{r}}^{(1)} \cos \theta_{\mathbf{r}}^{(2)}, \quad S_{\mathbf{r}}^y = \sin \theta_{\mathbf{r}}^{(1)} \cos \theta_{\mathbf{r}}^{(2)}, \quad S_{\mathbf{r}}^z = \sin \theta_{\mathbf{r}}^{(2)}, \quad (2)$$

with $-\pi \leq \theta^{(1)} < \pi$, $-\frac{\pi}{2} \leq \theta^{(2)} < \frac{\pi}{2}$. Note that the variables chosen are just slightly modified angles φ, θ of the spherical coordinates $\theta_{\mathbf{r}}^{(1)} = \varphi, \theta_{\mathbf{r}}^{(2)} = \theta - \pi/2$, respectively.

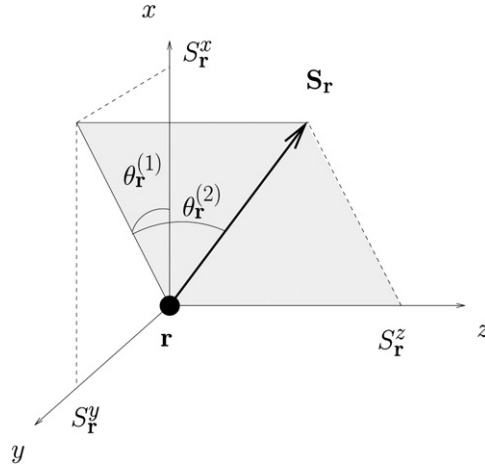


Figure 1. The angle variables $\theta_{\mathbf{r}}^{(1)}$ and $\theta_{\mathbf{r}}^{(2)}$ that can be used to define the position of the spin $\mathbf{S}_{\mathbf{r}}$ placed at the site \mathbf{r} .

Assuming that the angles $\theta_{\mathbf{r}}^{(1)}$, $\theta_{\mathbf{r}}^{(2)}$ are small at low temperatures for all spins of the system, this choice of coordinates enables us to substitute the scalar product of two spins that stands in (1):

$$\begin{aligned} S_{\mathbf{r}}^x S_{\mathbf{r}'}^x + S_{\mathbf{r}}^y S_{\mathbf{r}'}^y + S_{\mathbf{r}}^z S_{\mathbf{r}'}^z &= \cos(\theta_{\mathbf{r}}^{(1)} - \theta_{\mathbf{r}'}^{(1)}) \cos(\theta_{\mathbf{r}}^{(2)} - \theta_{\mathbf{r}'}^{(2)}) \\ &+ (1 - \cos(\theta_{\mathbf{r}}^{(1)} - \theta_{\mathbf{r}'}^{(1)})) \sin \theta_{\mathbf{r}}^{(2)} \sin \theta_{\mathbf{r}'}^{(2)} \end{aligned} \quad (3)$$

by an expression quadratic in $\theta_{\mathbf{r}}^{(1)}$, $\theta_{\mathbf{r}}^{(2)}$. Thus, (3) can be written in the low-temperature approximation as

$$S_1^x S_2^x + S_1^y S_2^y + S_1^z S_2^z \approx 1 - \frac{1}{2}(\theta_1^{(1)} - \theta_2^{(1)})^2 - \frac{1}{2}(\theta_1^{(2)} - \theta_2^{(2)})^2, \quad (4)$$

and the Hamiltonian (1) is reduced to

$$H = H_0 + H_1^{XY}(\{\theta^{(1)}\}) + H_1^{XY}(\{\theta^{(2)}\}), \quad (5)$$

where

$$H_1^{XY}(\{\theta\}) = \frac{1}{4} \sum_{\mathbf{r}} \sum_{\mathbf{r}'} J(\mathbf{r} - \mathbf{r}') (\theta_{\mathbf{r}} - \theta_{\mathbf{r}'})^2 \quad (6)$$

is the Hamiltonian of the 2D XY model on the same lattice taken in the SWA [20]. H_0 can be regarded as a shift in the energy scale.

The spin-spin pair correlation function with the assumption about smallness of all $\theta_{\mathbf{r}}^{(1)}$, $\theta_{\mathbf{r}}^{(2)}$ reads

$$G_2(R) = \langle \mathbf{S}_{\mathbf{r}} \cdot \mathbf{S}_{\mathbf{r}+\mathbf{R}} \rangle \approx \langle \cos(\theta_{\mathbf{r}}^{(1)} - \theta_{\mathbf{r}+\mathbf{R}}^{(1)}) \cos(\theta_{\mathbf{r}}^{(2)} - \theta_{\mathbf{r}+\mathbf{R}}^{(2)}) \rangle, \quad (7)$$

where the angular brackets stand for the thermodynamic averaging:

$$\langle \dots \rangle = \frac{1}{Z} \text{Tr}(\dots e^{-\beta H}), \quad \text{with} \quad Z = \text{Tr} e^{-\beta H}$$

and

$$\text{Tr} \dots = \prod_{\mathbf{r}} \frac{1}{4\pi} \int_{-\pi}^{\pi} d\theta_{\mathbf{r}}^{(1)} \int_{-\pi/2}^{\pi/2} d\theta_{\mathbf{r}}^{(2)} \cos \theta_{\mathbf{r}}^{(2)} \dots \quad (8)$$

In the 2D XY model, the power-law decay of the spin–spin correlation function with distance serves as an indication of QLRO. A suitable quantity to characterize the decay of the correlation function with an increase of the distance R is the temperature-dependent exponent:

$$\eta(T) = - \lim_{R \rightarrow \infty} \frac{\ln G_2(R)}{\ln R}. \quad (9)$$

In the case of the 2D XY model, the SWA gives for the exponent η^{XY} [20]:

$$\eta^{XY} = 1/(2\pi\beta J) \quad (10)$$

that is reliable for small temperatures [21, 22].

Due to the separation of the angle variables $\theta_{\mathbf{r}}^{(1)}, \theta_{\mathbf{r}}^{(2)}$ in (5) and (7), we can write for the correlation function

$$G_2(R) = G_2^{(1)}(R) \times G_2^{(2)}(R), \quad (11)$$

where

$$G_2^{(1)}(R) = \frac{1}{Z_1} (2\pi)^{-N} \left(\prod_{\mathbf{r}'} \int_{-\pi}^{\pi} d\theta_{\mathbf{r}'}^{(1)} \right) e^{-\beta H_1^{XY}(\{\theta^{(1)}\})} \cos(\theta_{\mathbf{r}}^{(1)} - \theta_{\mathbf{r}+\mathbf{R}}^{(1)}) \quad (12)$$

and

$$G_2^{(2)}(R) = \frac{1}{Z_2} 2^{-N} \left(\prod_{\mathbf{r}'} \int_{-\pi/2}^{\pi/2} d\theta_{\mathbf{r}'}^{(2)} \cos \theta_{\mathbf{r}'}^{(2)} \right) e^{-\beta H_1^{XY}(\{\theta^{(2)}\})} \cos(\theta_{\mathbf{r}}^{(2)} - \theta_{\mathbf{r}+\mathbf{R}}^{(2)}). \quad (13)$$

Z_1 and Z_2 respectively originate from the integration over $\theta_{\mathbf{r}}^{(1)}$ and $\theta_{\mathbf{r}}^{(2)}$ in the partition function $Z = Z_1 Z_2$. Although it may be believed that the low-temperature approximation applied to $O(n)$ models automatically leads to the $(n-1)\eta^{XY}$ exponent, the presence of the cosine in the integration element in (13) makes the problem more involved.

Now, to define the decay of the spin–spin correlation function $G_2(R)$ for large distances R , it is enough to find the asymptotic behaviour of $G_2^{(1)}(R)$ and $G_2^{(2)}(R)$ in the limit $R/a \rightarrow \infty$. It is easy to see that $G_2^{(1)}(R)$, equation (12), is just the correlation function of the 2D XY model, $G_2^{XY}(R)$, the asymptotic behaviour of which is well known:

$$G_2^{(1)}(R) = G_2^{XY}(R) \approx (R/a)^{-\eta^{XY}} \quad (14)$$

with η^{XY} given by (10). So, the problem is to evaluate $G_2^{(2)}(R)$. We will follow the same scheme that has been used to find $G_2^{XY}(R)$ [20]. For this purpose we pass to the Fourier variables

$$\theta_{\mathbf{r}}^{(2)} = \frac{1}{L} \sum_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}} \theta_{\mathbf{k}}, \quad \theta_{\mathbf{k}} = \frac{1}{L} \sum_{\mathbf{r}} e^{-i\mathbf{k}\mathbf{r}} \theta_{\mathbf{r}}^{(2)}, \quad (15)$$

where \mathbf{r} spans the sites of a square lattice $L \times L$ and \mathbf{k} spans the first Brillouin zone in the corresponding Fourier space. Then the Hamiltonian (6) reads

$$H_1^{XY}(\{\theta\}) = J \sum_{\mathbf{k} \neq 0} \gamma_{\mathbf{k}} \theta_{\mathbf{k}} \theta_{-\mathbf{k}}$$

with $\gamma_{\mathbf{k}} \equiv 2 - \cos k_x - \cos k_y$, and the Jacobian $\prod_{\mathbf{r}} \cos \theta_{\mathbf{r}}^{(2)}$ in (13) can be replaced in the low-temperature approximation by $\exp[-\frac{1}{2} \sum_{\mathbf{r}} (\theta_{\mathbf{r}}^{(2)})^2]$ and brought to the expression of the same type as the Boltzman factor $e^{-\beta H_1^{XY}}$ due to the equality $\sum_{\mathbf{r}} (\theta_{\mathbf{r}}^{(2)})^2 = \sum_{\mathbf{k}} \theta_{\mathbf{k}} \theta_{-\mathbf{k}}$. The

cosine $\cos(\theta_{\mathbf{r}}^{(2)} - \theta_{\mathbf{r}+\mathbf{R}}^{(2)})$ in (13) can be presented in the Fourier variables as the real part of

$$\exp\left[\frac{i}{L} \sum_{\mathbf{k}} (e^{i\mathbf{k}(\mathbf{r}+\mathbf{R})} - e^{i\mathbf{k}\mathbf{r}})\theta_{\mathbf{k}}\right].$$

Thus, (13) comes to a product of integrals of the type $\int d\theta e^{-a\theta^2+b\theta}$, easily integrable if the boundaries of integration are extended to infinity that can be considered as a nice approximation in the low-temperature limit (since $a \sim 1/T$). The integration gives

$$G_2^{(2)}(R) = \exp\left(-\frac{1}{\beta J N} \sum_{\mathbf{k}} \frac{\sin^2 \frac{\mathbf{k}\mathbf{R}}{2}}{\gamma_{\mathbf{k}} + \frac{1}{2\beta J}}\right). \tag{16}$$

To discover the concurrent dependence of (16) on the temperature βJ and the distance R/a when these two parameters are large numbers we approximate $\gamma_{\mathbf{k}}$ for small \mathbf{k} as $k^2/2$, and pass from the sum to an integral using polar coordinates $\frac{1}{2}\mathbf{k}\mathbf{R} = \frac{1}{2}kR \cos \varphi \equiv z \cos \varphi$

$$I(R) \equiv \frac{1}{N} \sum_{\mathbf{k}} \frac{\sin^2 \frac{\mathbf{k}\mathbf{R}}{2}}{\gamma_{\mathbf{k}} + \frac{1}{2\beta J}} = \frac{1}{2\pi^2} \int_0^{\frac{\sqrt{\pi}}{a}R} \frac{z dz}{z^2 + \frac{(R/a)^2}{4\beta J}} \int_0^{2\pi} d\varphi \sin^2(z \cos \varphi). \tag{17}$$

In the limit $\frac{(R/a)^2}{4\beta J} \gg 1$, $\sin^2(z \cos \varphi)$ can be replaced by its average $\frac{1}{2}$ leading to $I(R) \approx \frac{1}{2\pi} \ln(4\pi\beta J)$. In the other limit $\frac{(R/a)^2}{4\beta J} \ll 1$, we choose a finite parameter $\varepsilon < 1$ such that $\frac{(R/a)^2}{4\beta J} / \varepsilon^2$ is still small, then split $I(R)$ into two integrals $\int_0^\varepsilon + \int_\varepsilon^{\frac{\sqrt{\pi}}{a}R}$. The first one can be shown after expansion of the sine and term-by-term integration to vanish in the present limit while the second one has leading behaviour $\frac{1}{2\pi} \ln(R/a)$. Eventually, we obtain

$$G_2^{(2)}(R) \approx (R/a)^{-\frac{1}{2\pi\beta J}} \quad \text{for} \quad \frac{(R/a)^2}{4\beta J} \ll 1 \tag{18}$$

and

$$G_2^{(2)}(R) \approx (4\pi\beta J)^{-\frac{1}{2\pi\beta J}} \quad \text{for} \quad \frac{(R/a)^2}{4\beta J} \gg 1. \tag{19}$$

Thus, $G_2^{(2)}(R)$ is either constant with respect to R or equivalent to (14) depending on the value of the ratio $\frac{(R/a)^2}{4\beta J}$.

Substituting (18), (19) into (11) with the known expression for $G_2^{(1)}(R)$, equation (14), we get the following behaviour of the spin–spin correlation function:

$$G_2(R) \approx (R/a)^{-2\eta^{XY}} \quad \text{for} \quad \frac{(R/a)^2}{4\beta J} \ll 1, \tag{20}$$

$$G_2(R) \approx (4\pi\beta J)^{-\eta^{XY}} (R/a)^{-\eta^{XY}} \quad \text{for} \quad \frac{(R/a)^2}{4\beta J} \gg 1. \tag{21}$$

Let us clarify which of the above two estimates corresponds to the behaviour observable in practice. An approach used in the above derivations was based on the assumptions about smallness of the temperature and finiteness of the lattice. Therefore, the limit $\beta J \rightarrow \infty$ is physically grounded, because the lower the temperature we consider, the more the likely ordering in the system is. But the limit $R/a \rightarrow \infty$ as well as $L \rightarrow \infty$ used to obtain approximate estimates of the integrals in practice is limited by finiteness of the lattice: $R/a < L$. As the lattice size grows to infinity, the ordering disappears and our approach may become invalid. From the above arguments, we conclude that for a system of a finite size

in the low-temperature limit the estimate (20) holds. Moreover, power-law asymptotics (20), (21) brings about QLRO present in the system. Recall that these formulae were obtained by means of the low-temperature approximation. Applicability of the latter to the 2D Heisenberg model has been justified at the beginning of this paper by a finite-size system that leads to residual magnetization at low T . Therefore, although the QLRO was not considered as an intrinsic property of a finite-size system, the power-law asymptotics (20), (21) gives arguments in favour of its presence.

Let us quote another argument that favours the QLRO in the 2D Heisenberg model, which by no means is connected to the low-temperature approximation and holds also for an infinite system. In [14] arguments were given that the model undergoes a freezing transition at non-zero temperature [12] with typical low-temperature configurations in the form of a gas of super-instantons [11]. Subsequently, an onset of the low-temperature QLRO phase is characterized by the power-law decay of the pair correlation function with an exponent $\eta = \eta^{XY}$ [13, 14]. The temperature range where one would expect to observe the behaviour (21) is thus already dominated by the defects, and our approximation fails. Note also that our result (20) does not contradict the estimate of [13], since the former is valid at low temperatures, whereas the latter holds at the transition temperature. Although our approach cannot give a definite answer about the presence of QLRO phase in an infinite system, this question is still under discussion.

To verify our analytic results, we have performed Monte Carlo simulations of the Heisenberg spin model on lattices of different sizes (with periodic boundary conditions) and at different temperatures. Wolff's cluster algorithm was used for this purpose [23]. The exponent η is obtained on the base of three different observables, analysing the finite-size scaling (FSS) of the magnetization, $M \sim L^{-\frac{1}{2}\eta(T)}$, the pair correlation function, $G_2(L/2) \sim (L)^{-\eta(T)}$, and the magnetic susceptibility, $\chi \sim L^{2-\eta(T)}$. Note that we use the FSS behaviour for the correlation function rather than the distance dependence, since the boundary conditions introduce complicated scaling functions which spoil the expected algebraic decay [22]. All three quantities are computed at different temperatures for varying system sizes, giving access to a temperature-dependent exponent $\eta(T)$. Power-law scaling found for all three quantities M , G_2 and χ supports the presence of a QLRO phase found by analytic considerations. The lattice size in our simulations changes from $N = 8 \times 8$ to $N = 256 \times 256$ for each fixed temperature (figure 2) in order to obtain the FSS estimates of $\eta(T)$, as shown in figure 3. Note that almost all the data follow from magnetization measurements, since susceptibility and correlation function are subject to stronger fluctuations and would require much longer simulations. We cover the range of temperatures from 10^{-9} to the order of 1. Thus in fact we observe both cases $\frac{(R/a)^2}{4\beta J} \ll 1$ and $\frac{(R/a)^2}{4\beta J} \gg 1$. However, comparing the analytic results and the outcome of our Monte Carlo simulations in figure 3, we see that $\eta = 2\eta^{XY}$ fits the Monte Carlo data over the whole range of temperatures except the last several points (at the high temperature side of the window shown in figure 3) which must indicate a transition to a non-algebraic behaviour (see [13] and [24]). Thus, η defined by (21) has not been observed in our computer simulations. The natural conclusion is that when the condition $\frac{(R/a)^2}{4\beta J} \gg 1$ is reached, the temperature is not low enough to use our approach and possibly is already close to the conjectured transition temperature of the model (the estimate is shown in figure 2 as the intersection of dotted lines, see [12]). Hence, the question about the possibility of observing (21) in MC simulations remains open. But the important conclusion of the work is that the result $\eta = 2\eta^{XY}$ for the Heisenberg model in two dimensions is reliable in a wide range of low temperatures up to lattices 256×256 .

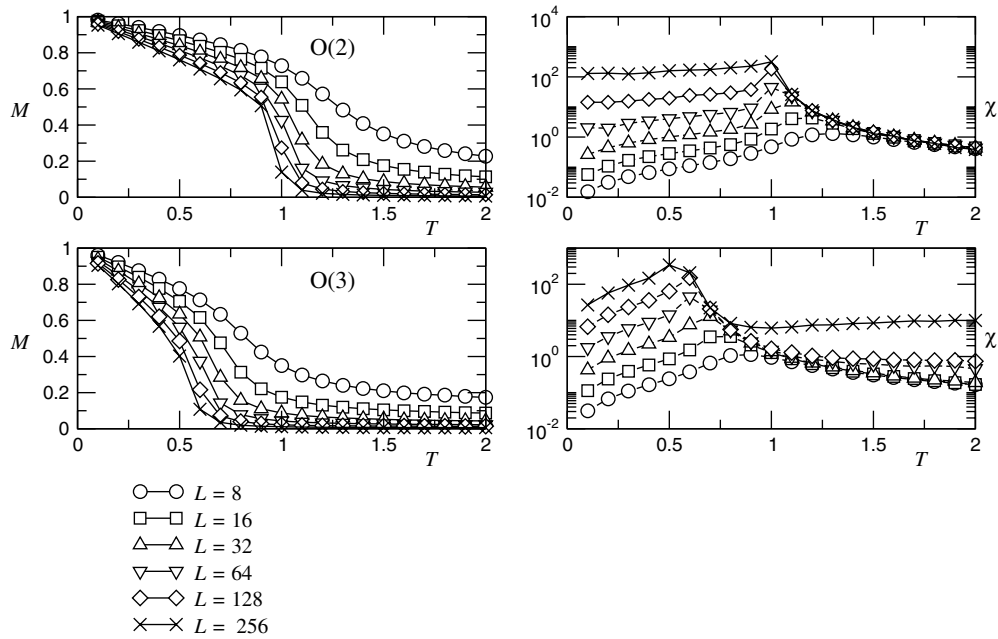


Figure 2. Monte Carlo results for XY ($O(2)$) (to illustrate the well-established case) and Heisenberg ($O(3)$) models for finite two-dimensional lattices of different sizes.

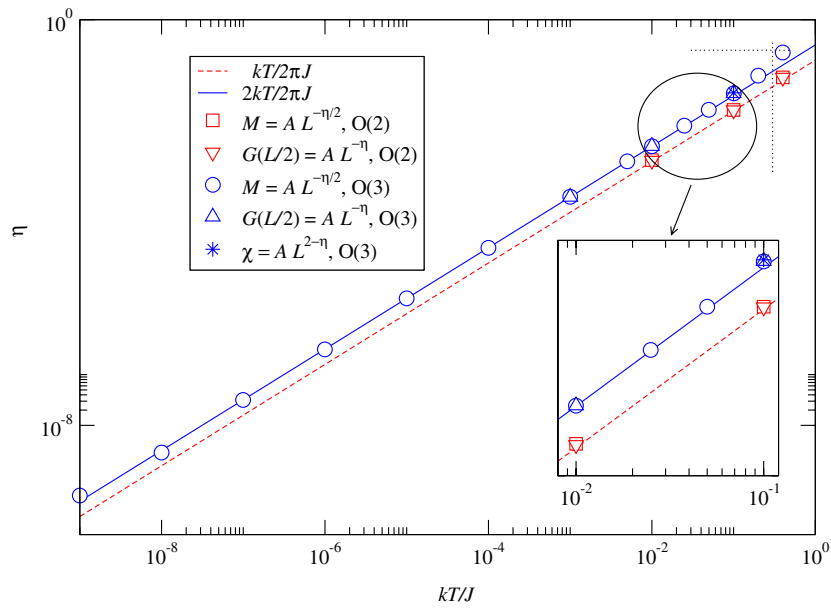


Figure 3. A comparison between the exponents η of the Heisenberg model obtained from the Monte Carlo simulations and from the analytic calculation in the low-temperature approximation. The dashed line presents η^{XY} . The inset shows an increase of the scale to make the different symbols used more visible.

(This figure is in colour only in the electronic version)

Acknowledgments

We acknowledge the CNRS-NAS exchange programme and Loïc Turban and Dragi Karevski for a discussion of the results. We thank Erhard Seiler for useful correspondence.

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