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

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Abstract. We analyse the low-temperature behaviour of the Heisenberg model on a two-dimensional lattice *of finite size*. Presence of a residual magnetisation in a finite-size system enables us to use the spin wave approximation, which is 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 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.

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The long history of the Heisenberg model in two dimensions is characterised by a competition between two contrary opinions about properties of this model. The early observation, made by Peierls [1], about long-wavelength lattice waves destroying the localisation 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 magnetisation 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 characterised by an order parameter in an 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, 6, 7]. This scenario is deeply connected to the symmetry of the model. In the XY model rotations of a spin form an Abelian group what allows formation of stable topological defects like 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, since no stable topological defects (instantons) can be formed. 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. Refs. [10, 11, 12, 13, 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*. And 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 well known now that in a finite $2D$ XY -spin system below the BKT transition temperature there is a non-vanishing magnetisation 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 Ref. [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 magnetisation, 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 $\mathbf{S}_{\mathbf{r}} = (S_{\mathbf{r}}^x, S_{\mathbf{r}}^y, S_{\mathbf{r}}^z)$ in the Hamiltonian of the Heisenberg model on a two-dimensional lattice 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 allows us to treat the model by means of the spin-wave approximation (SWA). We consider the case of the nearest neighbours interaction potential $J(\mathbf{r} - \mathbf{r}') = J\delta_{|\mathbf{r}-\mathbf{r}'|,a}$, and $1/2$ stands in (1) to prevent double count of each bond.

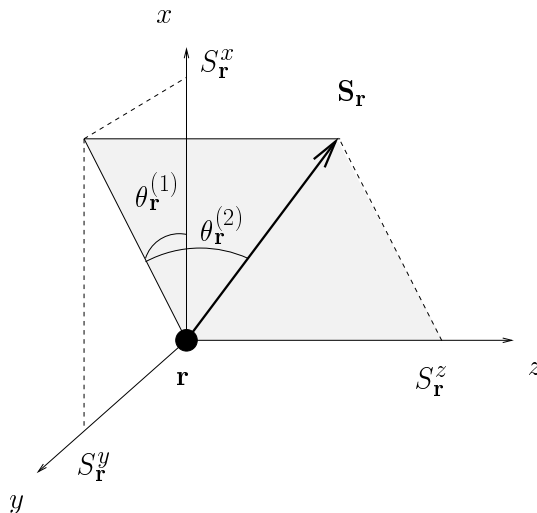


Figure 1. The angle variables $\theta_{\mathbf{r}}^{(1)}$ and $\theta_{\mathbf{r}}^{(2)}$ that can be used to define the position of the spin $\mathbf{S}_{\mathbf{r}}$ placed at the site \mathbf{r} .

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

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

with $-\pi < \theta^{(1)} < \pi$, $-\frac{\pi}{2} < \theta^{(2)} < \frac{\pi}{2}$. Note that the variables chosen are just slightly modified angles φ , θ of the spherical coordinates: $\theta_{\mathbf{r}}^{(1)} = \varphi$, $\theta_{\mathbf{r}}^{(2)} = \theta - \pi/2$. 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 make use of the SWA and to substitute the scalar product of two spins that stands in (1):

$$S_{\mathbf{r}}^x S_{\mathbf{r}'}^y + S_{\mathbf{r}}^y S_{\mathbf{r}'}^y + S_{\mathbf{r}}^z S_{\mathbf{r}'}^z = \cos(\theta_{\mathbf{r}}^{(1)} - \theta_{\mathbf{r}'}^{(1)}) \cos(\theta_{\mathbf{r}}^{(2)} - \theta_{\mathbf{r}'}^{(2)}) + \left(1 - \cos(\theta_{\mathbf{r}}^{(1)} - \theta_{\mathbf{r}'}^{(1)})\right) \sin \theta_{\mathbf{r}}^{(2)} \sin \theta_{\mathbf{r}'}^{(2)}, \quad (3)$$

by an expression quadratic in $\theta_{\mathbf{r}}^{(1)}$, $\theta_{\mathbf{r}}^{(2)}$. Thus, (3) can be written in the SWA 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 correlation function with the assumption about smallness of all $\theta_{\mathbf{r}}^{(1)}$, $\theta_{\mathbf{r}}^{(2)}$ reads:

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

where the angular brackets stand for the thermodynamic averaging:

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

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 characterise the decay of the correlation function with 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].

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

$$G_2^{(1)}(R) = \frac{1}{Z_1} (4\pi)^{-N} \left(\prod_{\mathbf{r}'} \int_{-\pi}^{\pi} d\theta_{\mathbf{r}'}^{(1)} \right) e^{-\beta H_1^{XY}(\{\theta^{(1)}\})} \cos(\theta_{\mathbf{r}}^{(1)} - \theta_{\mathbf{r}+\mathbf{R}}^{(1)}) \quad (12)$$

and

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

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 SWA applied to $O(n)$ models automatically leads to $(n-1)\eta^{XY}$ 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 $G_2^{(1)}(R)$, Eq.(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:

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

where N is the total number of lattice sites and \mathbf{k} spans the 1st Brillouin zone. 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 $\gamma_{\mathbf{k}} \equiv 2 - \cos k_x a - \cos k_y a$, and the integration in (13) must be changed to

$$\left(\prod_{\mathbf{k} \in B/2} \int_{-\infty}^{\infty} d\theta_{\mathbf{k}}^c \int_{-\infty}^{\infty} d\theta_{\mathbf{k}}^s \right) \quad (16)$$

with the product taken over a half of the 1st Brillouin zone denoted by $B/2$. The cosine $\cos(\theta_{\mathbf{r}}^{(2)} - \theta_{\mathbf{r}+\mathbf{R}}^{(2)})$ in (13) can be presented in the Fourier variables as

$$\text{Re} \exp \left[\frac{i}{\sqrt{N}} \sum_{\mathbf{k} \neq 0} (\eta_{\mathbf{k}}^c \theta_{\mathbf{k}}^c + \eta_{\mathbf{k}}^s \theta_{\mathbf{k}}^s) \right]$$

with $\eta_{\mathbf{k}}^c = \cos \mathbf{k}\mathbf{r} - \cos \mathbf{k}(\mathbf{r} + \mathbf{R})$ and $\eta_{\mathbf{k}}^s = -(\sin \mathbf{k}\mathbf{r} - \sin \mathbf{k}(\mathbf{r} + \mathbf{R}))$. The product of cosines in (13) can be expressed in the SWA as

$$\prod_{\mathbf{r}} \cos \theta_{\mathbf{r}}^{(2)} \approx \prod_{\mathbf{r}} e^{-\frac{1}{2}(\theta_{\mathbf{r}}^{(2)})^2} = \exp \left[-\frac{1}{2} \sum_{\mathbf{r}} (\theta_{\mathbf{r}}^{(2)})^2 \right], \quad (17)$$

using the equality $\sum_{\mathbf{r}} (\theta_{\mathbf{r}}^{(2)})^2 = \sum_{\mathbf{k} \neq 0} \theta_{\mathbf{k}} \theta_{-\mathbf{k}}$ we obtain an integrable form for $G_2^{(2)}(R)$. After simple integration we have

$$G_2^{(2)}(R) = \exp \left(-\frac{1}{\beta J N} \sum_{\mathbf{k} \neq 0} \frac{\sin^2 \frac{\mathbf{k}\mathbf{R}}{2}}{\gamma_{\mathbf{k}} + \frac{1}{2\beta J}} \right). \quad (18)$$

Recall that we are interested in the long-distance behaviour of the pair correlation function (7) at low T . We estimate the asymptotic behaviour of (18) in the limit $R/a \rightarrow \infty$, $\beta J \rightarrow \infty$ for two cases:

$$G_2^{(2)}(R) \sim \begin{cases} (1 + 4\pi\beta J)^{-\frac{1}{2\pi\beta J}} & \text{for } \frac{(R/a)^2}{4\beta J} \gg 1; \\ (R/a)^{-\frac{1}{2\pi\beta J}} & \text{for } \frac{(R/a)^2}{4\beta J} \ll 1. \end{cases} \quad (19)$$

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

Substituting (19) into (11) with the known expression for $G_2^{(1)}(R)$, Eq.(12), we get the following asymptotic behaviour of the spin-spin correlation function:

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

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

Let us clarify which of the two above 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 temperature we consider, the more likely ordering in the system is. But the limit $R/a \rightarrow \infty$ as well as $N \rightarrow \infty$ used to obtain approximate estimates of the integrals in practice is limited by finiteness of the lattice: $(R/a)^2 < N$. 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 formulas were obtained by means of the SWA. Applicability of the latter to 2D Heisenberg model has been justified at the beginning of this paper by a finite system size that leads to residual magnetisation 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 SWA and holds also for an infinite system. In Refs. [14] arguments were given that the model undergoes a freezing transition at non-zero temperature [12] with typical low-temperature configurations in a form of a gas of superinstantons [11]. Subsequently, an onset of the low-temperature QLRO phase is characterised by the power-law decay of the pair correlation function with an exponent $\eta = \eta^{XY}$ [13, 14]. Note, 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 can not give a definite answer about the presence of QLRO phase in an infinite system, this question is still under discussion.

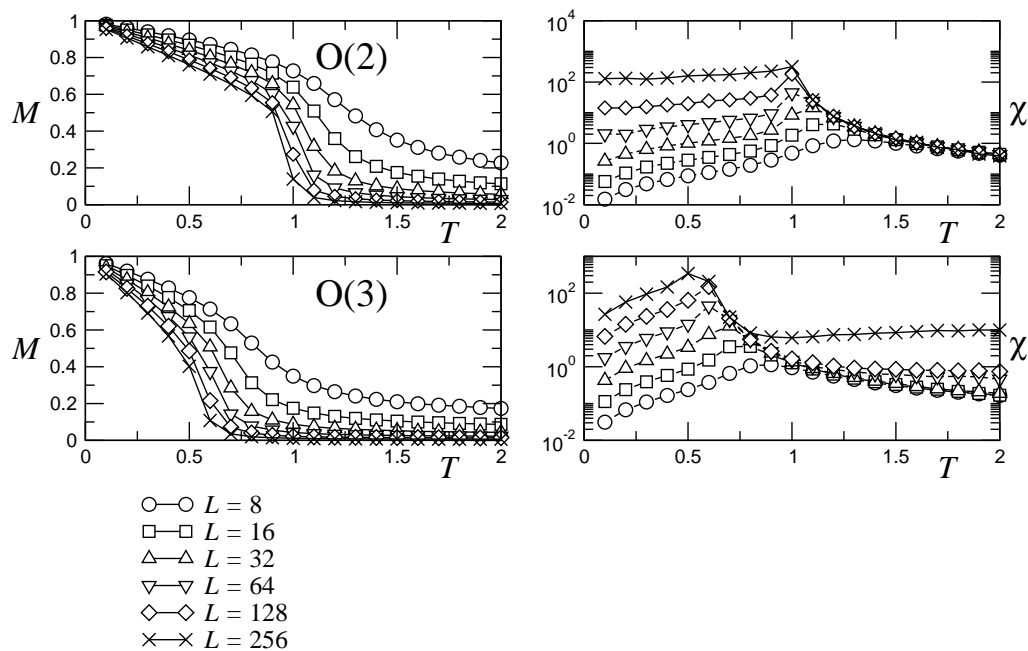


Figure 2. Monte Carlo results for XY (to illustrate the well established case) and Heisenberg models for finite two-dimensional lattices of different sizes.

To verify our analytic results we have performed Monte Carlo simulations of the Heisenberg spin model on lattices of different sizes and at different temperatures. The Wolff's cluster algorithm was used for this purpose [22]. The exponent η is obtained on the base of three different observables, analysing the finite-size scaling of the magnetisation, $M \sim L^{-\frac{1}{2}\eta(T)}$, the pair correlation function, $G_2(L/2) \sim (L)^{-\eta(T)}$ and the magnetic susceptibility, $\chi \sim L^{2-\eta(T)}$. 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. Note that the lattice size in our simulations changes from $N = 8 \times 8$ to $N = 256 \times 256$ for each fixed temperature (Fig. 2) in order to obtain the finite-size scaling estimates of $\eta(T)$ shown in Fig. 3. 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 Fig.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 Fig. 3) which must indicate a transition to a non algebraic behaviour (see Refs. [23] and [13]). Thus, η defined by (21) have 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 the approach based on the SWA and possibly is already close to the conjectured transition temperature of the model (see Refs. [12]). Hence, the question about a possibility to observe (21) in MC simulations remains opened. 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 .

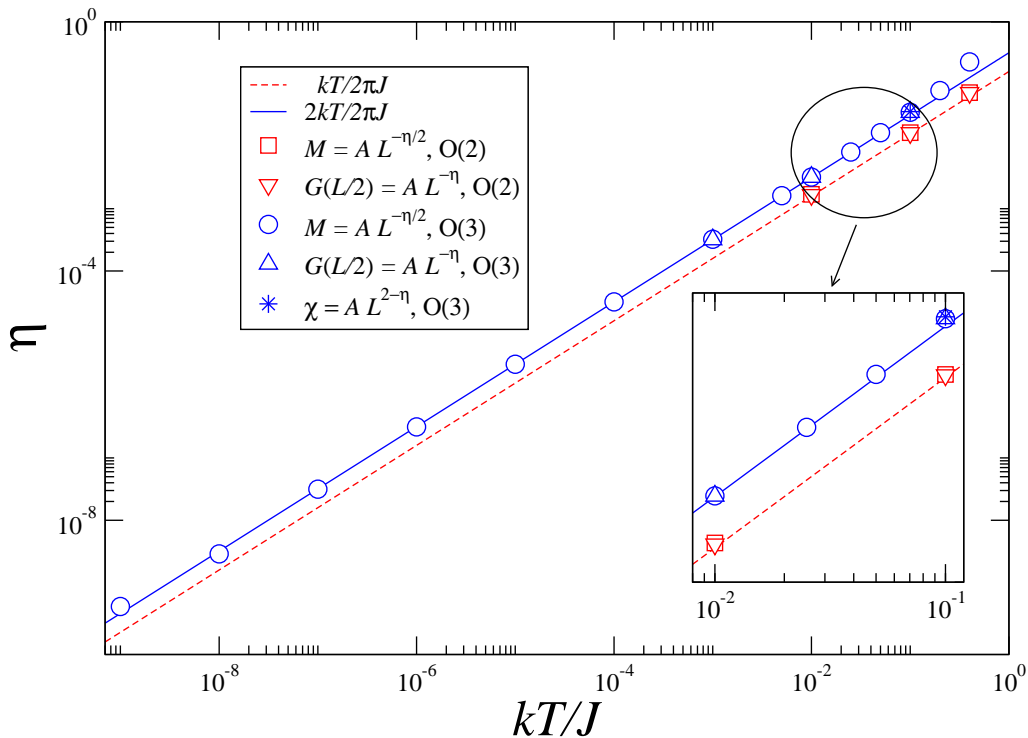


Figure 3. Comparison between the exponents η of the Heisenberg model obtained from the Monte Carlo simulations and from the analytic calculation in the SWA. The dashed line presents η^{XY} . The inset shows an increase of the scale to make the different symbols used more visible.

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