Monte Carlo calculation of the spin-stiffness of the two-dimensional Heisenberg model

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Abstract

Using a collective-mode Monte Carlo method (the Wolff-Swendsen-Wang algorithm), we compute the spin-stiffness of the two-dimensional classical Heisenberg model. We show that it is the relevant physical quantity to investigate the behaviour of the model in the very low temperature range inaccessible to previous studies based on correlation length and susceptibility calculations.

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As well-known, the long-distance, low-energy physics of two-dimensional spin systems are expected to be obtained from a low-temperature perturbative expansion of a suitable Non Linear Sigma (NLσ) model. However, the relevance of the low-temperature expansion beyond perturbation theory relies on the assumption of asymptotic freedom. Although this property is hardly questionable for symmetric $O(N)/O(N-1)$ models with $N > 2$ (see however [1]) no definite answer is known for more general models, in particular for Non-Symmetric models such as $O(3) \otimes O(2)/O(2)$ which are relevant for the study of frustrated Heisenberg spin systems [2]. Indeed, these models are suspected to be strongly affected by topological excitations [3] which is a possible source of failure of the low-temperature expansion. In order to have a non perturbative control of the low-temperature expansion, one can take advantage of Monte Carlo simulations. Up to now, calculations have been mainly concerned with correlation lengths and susceptibilities [4]. Unfortunately, because of their exponential behaviour as a function of $\beta = 1/kT$ and the computationally accessible lattice sizes, studying the very low temperature regime is very demanding, or even impossible. The aim of this paper is to show that the relevant physical quantity allowing to reach this regime for accessible sizes is the spin-stiffness $\rho_s$, a measure of the free energy increment under twisting of the boundary conditions [3]. In the following we shall restrict ourselves to the two-dimensional classical Heisenberg model; applications to more involved models will be presented in a forthcoming work.

The Hamiltonian of the Heisenberg model is:

$$H = -J \sum_{<ij>} S_i \cdot S_j$$  \hspace{1cm} (1)

where $<ij>$ denotes the summation over nearest-neighbours of a finite square lattice of size $L$. In (1), $S_i$ are three-component unit-length classical vectors and $J$ is positive. Each site $i$ of the lattice is indexed by two coordinates $x_i$ and $y_i$.

We impose a twist in the $x$ direction, by coupling the system with two walls of spins: $S(x=0) = S_1$, $S(x=L) = S_2$, $S_2$ being deduced from $S_1$ by a rotation of angle $\theta$ around a direction $e$. The spin-stiffness $\rho_s$ is defined as:

$$\rho_s(L) = \left. \frac{\partial^2 F(\theta)}{\partial \theta^2} \right|_{\theta=0} .$$  \hspace{1cm} (2)

where $F$ is the free energy.

In terms of the spins it writes:

$$\rho_s(L) = \frac{J}{L^2} < \sum_{<ij>} (S_i \cdot S_j - S_i \cdot e S_j \cdot e) (x_i - x_j)^2 > -\frac{J}{T L^2} < (\sum_{<ij>} (S_i \wedge S_j) \cdot e) (x_i - x_j)^2 >$$  \hspace{1cm} (3)

where $T$ is the temperature and Boltzmann averages are performed with two walls of parallel spins fixed at boundaries in the $x$ direction.
The finite size behaviour of $\rho_s(L)$, when $L$ is much larger than the lattice spacing $a$ but much smaller than the correlation length $\xi$, has been calculated at one and two-loop order with use of the $O(3)/O(2)$ NL$\sigma$ model \[5,7\]:

$$\rho_s \sim \frac{1}{2\pi} \ln \frac{\xi}{L} + \frac{1}{2\pi} \ln \ln \frac{\xi}{L}$$

(4)

where the common coefficient $1/2\pi$ in front of the leading and sub-leading logarithmic terms is a universal number which is not modified by higher orders in the low-temperature expansion.

The crucial point in measuring $\rho_s$ is that its predicted size dependence given by (4) is all the more valid since $L \ll \xi$. Therefore, in the very low temperature regime we can hope to test formula (4) by using a large range of relatively small lattice sizes. In contrast, measuring the temperature dependence of $\xi$ requires $\xi \leq L$ and therefore relatively high temperatures for accessible sizes\[4\], a regime where the validity of the perturbation theory becomes less controlled. A most important point to notice is that at the very low temperatures considered here the physics of the model is entirely controlled by collective excitations - spin waves- and therefore we must take great care of these large-scale moves in any simulation of the model ("beating" the critical slowing down).

The purpose of this paper is to present a Monte Carlo study of the spin-stiffness for the finite two-dimensional classical Heisenberg model free of critical slowing down and then to investigate numerically prediction (4). To summarize what have been obtained, our Monte Carlo calculations confirm the existence of a leading logarithmic contribution with the universal amplitude $1/2\pi$. In addition, an extra-contribution to the spin-stiffness consistent with the subleading term of (4) has also been clearly identified. The Monte Carlo results presented have been obtained using the Wolff-Swendsen-Wang method \[8\] of updating large clusters of spins simultaneously. At the low temperatures considered here, using a collective Monte Carlo algorithm appeared to be essential to get well-converged values of the spin-stiffness. In particular, our preliminary attempts making use of a Monte Carlo algorithm based on local spin updates failed due to the severe critical slowing down.

To our knowledge, we present the first unambiguous numerical calculation validating the precise finite-size behavior of the spin-stiffness of the two-dimensional classical Heisenberg model. It should be noted that a similar calculation has been reported recently by Mon \[9\]. However, we disagree both with the theoretical expression of the spin-stiffness used by the author and with the relevance of the local Monte Carlo scheme employed in his work.

**Results.** The Wolff-Swendsen-Wang (WSW) algorithm has been implemented to simulate the Heisenberg model on a $L \times L$ square lattice. In the y-direction periodic boundary conditions have been chosen. In the x-direction, fixed boundary conditions are to be used. Whereas in a
local Monte Carlo algorithm imposing fixed walls of spins pointing in some given direction is elementary, the situation is different when clusters of spins are built with WSW. To escape from this difficulty we have also chosen periodic boundary conditions in the x-direction. This introduces an error in the spin-stiffness exponentially small in ln \( L \). As expected, this contribution has been found to play no role in the following finite-size analysis. We have found that relatively moderate sizes \( L \) are in fact sufficient to validate formula (4). Lattices of sizes \( L = 4, 8, 12, \ldots, 32 \) have been simulated. We have performed our simulations at four different temperatures: \( T/J = 0.1, 0.15, 0.3, \) and 0.395. In each case we are at sufficiently low temperature to be in the regime of validity of formula (4) (\( L \ll \xi \)).

Figure 1 presents the complete set of results obtained for the spin-stiffness at different sizes and temperatures. At the scale of Figure 1, all curves appear to be very rapidly linear as a function of ln \( L \). In order to determine accurately the corresponding slope a closer look is necessary. Figure 2 presents a blow up of data of Figure 1 for the lowest (upper figure) and highest (lower figure) temperatures treated, \( T/J = 0.1 \) and \( T/J = 0.395 \), respectively. A first point to notice is that a very high accuracy on our data has been achieved. Such a level of accuracy is absolutely necessary to put into evidence the linear regime of the spin-stiffness as well as to get a truly converged estimate of the slope. We emphasize that only when resorting to a collective Monte Carlo scheme we have been able to fulfill both requirements. In our first attempts to use a local Monte Carlo scheme we observed a systematic and uncontrolled long-term drift of the estimates of the statistical mean values. A first important remark concerning Figure 2 is how fast we enter the linear regime: at all temperatures considered it is reached at \( L \sim 16 \). By using data for \( L = 16, 20, 24, 28, \) and 32 an estimate of the slope can be extracted, we get: -0.162(4), -0.166(5), -0.171(5), and -0.184(7) at \( T/J = 0.1, 0.15, 0.3, \) and 0.395, respectively. At the very low temperature \( T/J = 0.1 \) we recover within statistical fluctuations the theoretical result \( 1/2\pi = 0.1592\ldots \) predicted by formula (4). At higher temperatures non-negligible higher-order contributions in the spin-stiffness show up. To put this on a more quantitative basis, we have performed a fit of the data using the full expression (4). The resulting curve is represented by a solid line in Figure 2. The only free parameter entering the fit is the correlation length \( \xi \), the arbitrary reference value for the spin-stiffness being chosen so as to reproduce exactly the last data (\( L = 32 \)). The dashed line is the linear curve obtained when resorting to the leading logarithmic behaviour (no ln ln corrections, no renormalization of the \( 1/2\pi \) slope) using the very same correlation length as determined in the fit. At \( T/J = 0.1 \), both curves almost coincide in the linear regime, illustrating the correctness of the leading log prediction and the smallness of the higher-order corrections at this temperature. At the higher temperatures considered, we clearly see the necessity of going beyond leading order. In addition, it is striking to see how good representation (4) is in reproducing our Monte Carlo data. Of course, at the accuracy determined by statistical fluctuations it is not realistic to
hope to resolve the precise analytical ln ln behavior of the second-order theoretical expression. However, our data are perfectly consistent with the “renormalized slope” predicted by (4),

\[ s^* = \partial \rho_s / \partial \ln L = -1/2\pi (1 + 1/\ln(\xi/L)). \]

In Figure 3 we have plotted the correlation length \( \xi \) issued from the fit using formula (4). We also present the curve obtained from the formula proposed by S.H. Shenker and J. Tobochnik [11] (obtained by matching high- and low-temperature calculations):

\[ \xi \simeq 0.01 \exp \frac{2\pi J/T}{1 + 2\pi J/T} \tag{5} \]

It is very satisfactory to see that our rough estimates of \( \xi \) are in good agreement with this completely independent calculation of the correlation length.

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[10] In fact, at this temperature the slope is very slightly renormalized. Using Eqs.4,5 we get -0.162 instead of the bare value of -0.1592... However, both values are not distinguishable within statistical fluctuations.

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**Figure Captions**

**Fig.1** Spin-stiffness for different sizes and temperatures. Statistical fluctuations smaller than the size of crosses.

**Fig.2** Blow up of Fig.1 for $T/J = 0.1$ and $T/J = 0.395$. The solid line is the best fit using Eq.4, the dashed line the first-order prediction (no renormalization of the slope).

**Fig.3** Correlation length $\xi$. The solid line is obtained from Eq.5, the values indicated by crosses from the fit of our data using Eq.4.