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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.

As well known, the long-distance, low-energy physics of two-dimensional spin systems is expected to be obtained from a low-temperature perturbative expansion of a suitable non-linear sigma (NLσ) model. In order to have a non-perturbative control of this low-temperature expansion, one can take advantage of Monte Carlo simulations. Up to now, calculations have been mainly concerned with correlation lengths and susceptibilities [1]. 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: 1) to show that the relevant physical quantity allowing to reach this regime for accessible sizes in the spin stiffness ρ_s, a measure of the free-energy increment under twisting of the boundary conditions [2,3]; 2) to argue that it is essential to use a *non-local* Monte Carlo algorithm to get truly converged values of the spin stiffness in the very low-temperature regime; 3) to exhibit in the case of the two-dimensional classical Heisenberg model the quasi-perfect agreement between the Monte

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Carlo simulation of the spin model and the predictions of the corresponding non-linear sigma (NLσ) model; applications to more involved systems will be presented in a forthcoming work.

To our knowledge, two previous works have attempted to compute the spin stiffness of the Heisenberg model. However, they are either based on a wrong formula [4], or on the use of a local Monte Carlo scheme [4, 5] not suited at all to the problem as discussed in the following. In our opinion, we present here the first unambiguous numerical calculation validating the precise finite-size behaviour of the spin stiffness of the two-dimensional classical Heisenberg model.

The Hamiltonian of the Heisenberg model is

$$H = -J \sum_{\langle ij \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j \,, \tag{1}$$

where $\langle ij \rangle$ denotes the summation over nearest neighbours of a finite square lattice of size L. In (1), $\boldsymbol{S}_i$ 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 $\boldsymbol{x}$-direction, by coupling the system with two walls of spins: $\boldsymbol{S}(\boldsymbol{x}=0)=\boldsymbol{S}_1$, $\boldsymbol{S}(\boldsymbol{x}=\boldsymbol{L})=\boldsymbol{S}_2$, $\boldsymbol{S}_2$ being deduced from $\boldsymbol{S}_1$ by a rotation of angle θ around a direction $\boldsymbol{e}$. The spin stiffness ρ_s is defined as

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

where F is the free energy.

In terms of the spins it writes

$$\rho_s(L) = \frac{J}{L^2}\left\langle \sum_{\langle ij \rangle} (\boldsymbol{S}_i \cdot \boldsymbol{S}_j - \boldsymbol{S}_i \cdot \boldsymbol{e}\, \boldsymbol{S}_j \cdot \boldsymbol{e})(x_i - x_j)^2 \right\rangle - \frac{J^2}{TL^2}\left\langle \left(\sum_{\langle ij \rangle} (\boldsymbol{S}_i \wedge \boldsymbol{S}_j) \cdot \boldsymbol{e}(x_i - x_j) \right)^2 \right\rangle, \tag{3}$$

where T is the temperature and Boltzmann averages are performed with two walls of parallel spins fixed at boundaries in the $\boldsymbol{x}$-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 ξ, has been calculated at one- and two-loop order with use of the $O(3)/O(2)$ NLσ model [2, 6]:

$$\frac{\rho_s}{T} \sim \frac{1}{2\pi} \ln \frac{\xi}{L} + \frac{1}{2\pi} \ln \ln \frac{\xi}{L} \,, \tag{4}$$

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

The crucial point in measuring ρ_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 ξ requires $\xi \leqslant L$ and, therefore, relatively high temperatures for accessible sizes [1], 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 prediction (4) numerically. To summarize what has 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 [7] 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 a well-converged estimate of the slope of the spin stiffness as a function of the lattice size. 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.

At this point, it seems important to discuss in more detail the previous attempts of calculating the spin stiffness of the Heisenberg model. Apart from the paper of Mon [4] in which a wrong formula for ρ_s has been used (he has mistakenly used the spin stiffness formula of the XY case), another calculation by Ritchey [5] done with the correct formula and using a local Metropolis algorithm has been performed. We have redone entirely his calculations with the very same conditions (same lattice sizes, same temperatures, same number of Monte Carlo steps). As already emphasized, we realized soon that such calculations are hampered by a severe critical slowing-down. Instead of getting a slope of approximately -0.16 (*i.e.* $1/2\pi$) Ritchey obtained a value of approximately -0.12. At the lowest temperature he treated, the difference between both figures results in fact from the non-convergence of his estimate of the slope (very slow convergence, independent configurations are too scarce). It is interesting to note that this difference has been boldly interpreted elsewhere as taking its origin from cubic corrections to the scaling [8], corrections which in fact are negligible at the lowest temperature presented by Ritchey. In this paper, highly converged estimates of the slope of the spin-stiffness are presented. Cubic corrections to the β-function (*i.e.* $\ln\ln$ corrections in formula (4)) showing up at sufficiently high temperatures are also put into evidence (see fig. 2).

Results. – The Wolff-Swendsen-Wang (WSW) algorithm has been implemented to simulate the Heisenberg model on an $L \times L$ square lattice. In the y-direction periodic boundary conditions have been chosen. In the x-direction, fixed boundary conditions are to be used. However, for simplicity we have also chosen periodic boundary conditions in the x-direction. This introduces an error in the spin stiffness exponentially small in $\ln L$. By using a very recently proposed interpretation of Wolff-type algorithms as algorithms based on an embedding of Ising spins into continuous spins [9] it can be seen that fixed boundary conditions can be implemented by introducing a suitable external magnetic field in the underlying Ising model. We have implemented this idea and found that the errors in the calculated spin stiffness are indeed exponentially small (less than 0.5% relative error for lattice sizes with $L > 8$). No difference on the resulting slopes have been observed within statistical fluctuations.

One of the major results of this paper is 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 a 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 fig. 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 fig. 1 for the lowest (upper figure) and

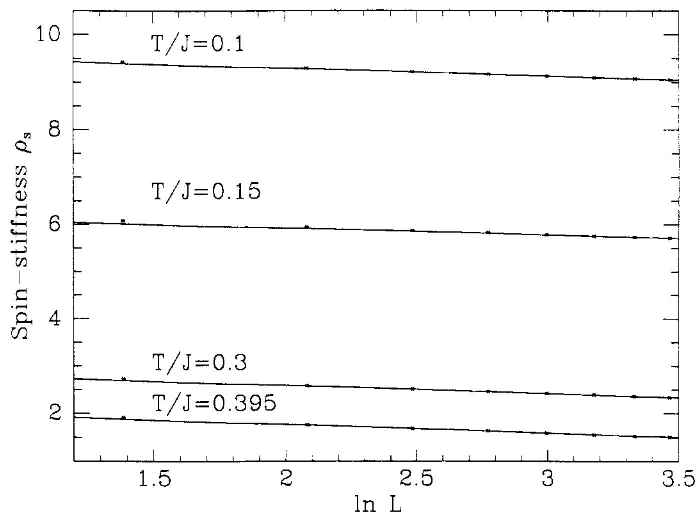

Fig. 1. – Spin stiffness for different sizes and temperatures. Statistical fluctuations smaller than the size of crosses.

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 fulfil both requirements. A first important remark concerning fig. 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) [1]. At higher temperatures non-negligible higher-order

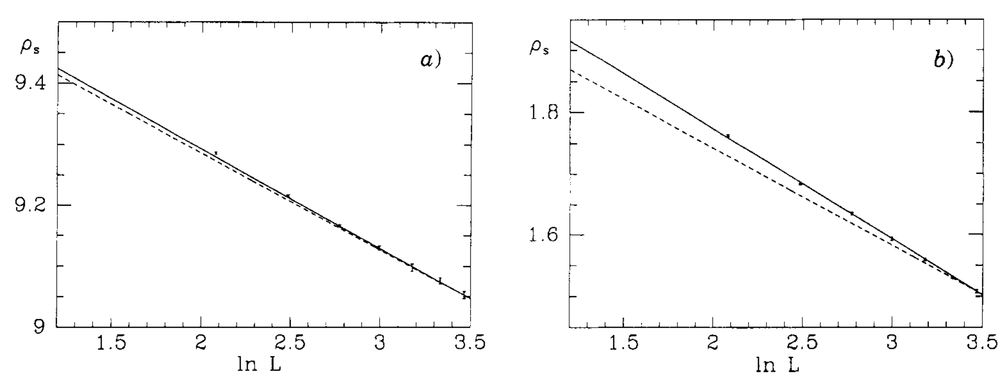

Fig. 2. – Blow-up of fig. 1 for $T/J = 0.1$ (a)) and $T/J = 0.395$ (b)). The solid line is the best fit using eq. (4), the dashed line the first-order prediction (no renormalization of the slope).

[1] 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.

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 fig. 2. The only free parameter entering the fit is the correlation length ξ, 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, due to the accuracy determined by statistical fluctuations and to the narrow range of lattice sizes used,it is not realistic to hope to resolve the precise analytical ln ln behaviour of the second-order theoretical expression. However, our data are perfectly consistent with the «renormalized slope» predicted by (4), $s^* = \partial(\rho_s/T)/\partial \ln L = -1/2\pi(1 + 1/\ln(\xi/L))$.

In fig. 3 we have plotted the correlation length ξ issued from the fit using formula (4). We also present the curve obtained from the formula proposed by Shenker and Tobochnik [10] (obtained by matching high- and low-temperature calculations):

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

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

In this paper, we have shown that for the case of the two-dimensional classical Heisenberg model it is possible to get a quasi-perfect agreement between the Monte Carlo simulation of the spin model and the predictions of the corresponding low-temperature non-linear sigma (NLσ) model. We have overemphasized that the essential point to obtain such a nice agreement is the use of an appropriate non-local Monte Carlo algorithm. The study of the spin siffness of more involved 2D systems such as frustrated Heisenberg spin models could be

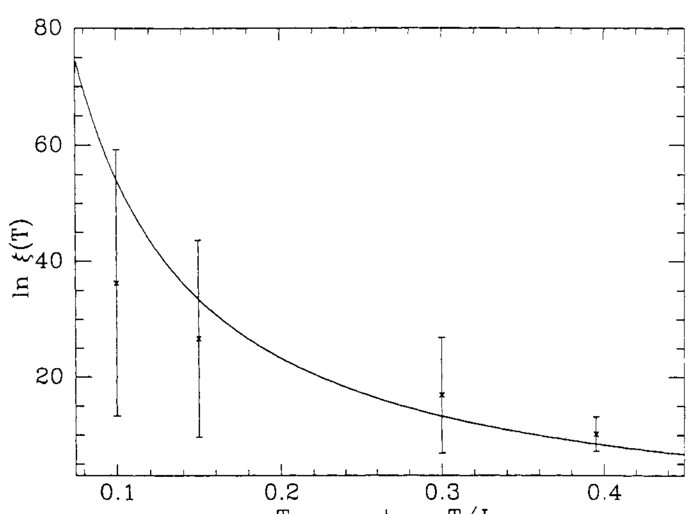

Fig. 3. – Correlation length ξ. The solid line is obtained from eq. (5), the values indicated by crosses from the fit of our data using eq. (4).

a very efficient test of the validity of the low-temperature perturbative expansion of the corresponding more general non-linear sigma models [11], an expansion which can be questioned due to the presence of non-trivial topological excitations [12] (2). However, the implementation of a non-local Monte Carlo scheme for such models is a highly non-trivial task; work in that direction is in progress.

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(2) Note that after completion of this work an interesting study of the spin stiffness for the case of a classical antiferromagnet on a triangular lattice using a local Monte Carlo scheme has been published [13].

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