Finite-size effects on the Hamiltonian dynamics of the XY-model

S. Lepri$^{1,2}$($^*$), S. Ruffo$^{1,2}$($^*$)

1 Dipartimento di Energetica “S. Stecco”, Via Santa Marta 3, I-50139 Florence, Italy
2 Istituto Nazionale di Fisica della Materia, Unità di Firenze, L.go E. Fermi 3 I-50125 Florence, Italy

PACS. 64.60.-i – General studies of phase transitions.
PACS. 64.60.Ht – Dynamic critical phenomena.

Abstract. – The dynamical properties of the finite-size magnetization $M$ in the critical region $T \leq T_{KB}$ of the planar rotor model on a $L \times L$ square lattice are analyzed by means of microcanonical simulations. The behavior of the $q = 0$ structure factor at high frequencies is consistent with field-theoretical results, but new additional features occur at lower frequencies. The motion of $M$ determines a region of spectral lines and the presence of a central peak, which we attribute to phase diffusion. Near $T_{KB}$ the diffusion constant scales with system size as $D \sim L^{-1.6(3)}$.

The XY or “planar rotor” model consists of a set of classical spins $S_r$ of unit length confined in a plane, whose orientation is specified by the angle $\theta_r$, $r$ being the position vector on a square lattice of size $N = L \times L$ with periodic boundary conditions. It is known that this model does not admit equations of motion and therefore its canonical dynamics is usually simulated either by Monte-Carlo methods [1, 2] or by Langevin type equations [3, 4]. Microcanonical approaches consist instead, either in considering a three component spin model [5] or into adding a kinetic energy term [6]. The latter method can be also generally applied to other physical systems (see e.g. the application to lattice gauge theories [3]). All these methods should display the same static properties, as it has been verified up to some extent [6, 8, 9].

One of the most striking features of the XY model is the presence of strong finite-size effects [10], e.g. the existence of a sizeable magnetization for large samples, despite the fact that long-range order cannot occur for the infinite system. For this reason, we are motivated to study the dynamical features of a finite lattice, a topic which has been far less investigated. In this respect the choice of the dynamics, e.g. canonical vs. microcanonical, is expected to play a crucial role.

In this Letter we consider the following Hamiltonian

$$\mathcal{H} = \sum_r \frac{p_r^2}{2} + \sum_{\langle r,r' \rangle} \left( 1 - \cos(\theta_r - \theta_{r'}) \right),$$

(1)
where $p_r = \dot{\theta}_r$ is the angular momentum of the rotor and the sum ranges over the four nearest neighbors of site $r$. We have set both the inertia of the rotors and the ferromagnetic coupling constant to unity so that the only physical control parameter is the energy per spin $e = \mathcal{H}/N$. Actually, there is a second constant of the motion, the total angular momentum $P = \sum_r p_r$, whose choice affects the results in a trivial way. In the numerical simulations we set $P = 0$ to avoid global ballistic rotation.

A previous study of the static properties of (1) showed that the system undergoes a Kosterlitz-Thouless-Berezinskii (KTB) transition at $e = e_{KTB} \approx 1.0$ corresponding to a kinetic temperature $T_{KTB} \approx 0.89$, which is in agreement with the value 0.894(5) obtained in the canonical ensemble.

Here, we focus our attention on the statistical behaviour of the instantaneous complex magnetization $M = M_x + iM_y$, defined as

$$M = \frac{1}{L^2} \sum_r S_r = \frac{1}{L^2} \sum_r e^{i\theta_r} = m e^{i\psi},$$

in the ordered phase $e < e_{KTB}$. In this regime the phase $\psi$ is well defined, because $m$ is bounded away from zero. Moreover, $\langle m \rangle$ is a sizeable quantity and can be regarded as a pseudo (i.e. non-extensive) order parameter ($\langle \cdot \rangle$ denotes the ensemble average). Indeed, it vanishes only algebraically with system size, $\langle m \rangle = (2N)^{-k_B T/8\pi}$ in the spin-wave limit.

The numerical integration of the equations of motion is performed using the fourth-order McLahlan-Atela algorithm which is an explicit scheme constructed from a suitable truncation of the evolution operator that preserves the Hamiltonian structure. One of the major merits of symplectic algorithms is that the error on the energy does not increase with the length of the run. The chosen time step (0.01-0.05 in our units) ensures that in every simulation energy fluctuates around the prescribed value with a relative accuracy below $10^{-5}$.

The dynamics is fully characterized by the structure factor $S(q, \omega)$, i.e. the space-time Fourier transform of the the spin-spin correlation function (we assume translational invariance)

$$S(r, t) = \langle e^{i\theta_t(0)} \rangle.$$

Accordingly, the power spectrum of $M$ is proportional to the zero wavenumber ($q = 0$) structure factor

$$S(0, \omega) \propto \int_{-\infty}^{\infty} \langle |M(t)M^*(0)|^2 \rangle e^{i\omega t} dt = \langle |M(\omega)|^2 \rangle.$$

The dynamical finite-size scaling hypothesis suggests that this quantity should be written as $\langle |M(\omega)|^2 \rangle / AL^z = f(\omega L)$, where $A$ is the area below the spectrum. According to the theory by Nelson and Fisher (NF) we expect $z = 1$ in our case. Our numerical results are in good agreement with these predictions, see Fig. 1a. Moreover, the high-frequency part ($L\omega \gg 1$) displays a power-law decay over approximatively one decade. This is a prediction of NF theory which, relying on a hydrodynamic description, is expected to hold in this frequency range, corresponding to times much shorter than the typical transit time of a wave on the lattice. Obviously a cutoff frequency of order unity is imposed by the lattice discreteness. Although an accurate estimation of the decay exponent is difficult in such a narrow range, the available data are consistent with the predicted law $\omega^{-3+\eta}$ (with $\eta = k_B T/2\pi$), at least up to the energy where a significant density of vortex pairs appears. This is precisely the case at $e = 0.992$ where we found $\omega^{-2.5(6)}$ which is actually significantly different from the NF value 3 $- \eta$ with $\eta \approx \eta(T_{KTB}) = 1/4$. Notice that this result is somehow in contrast with the theoretical expectations as it corresponds to $\eta > 1/4$. Similar deviations are indeed
observed in the static case and are traced back to the presence of multiplicative logarithmic corrections. Unfortunately, even the most accurate numerical result are controversial and apparently in contrast with the theory (see [17] and references within for a thoughtful account on this issue). We thus limit ourselves to observe that, at variance with what is reported in the literature we find $\eta > 1/4$ in the critical region.

The additional structure present in the spectrum at lower frequencies is beyond the validity range of NF theory and is related to the long-time dynamics of $M$ for the finite lattice. Indeed, it has been previously observed, in both Monte-Carlo [13] and microcanonical [18] simulations, that $M$ fluctuates in time in the complex plane in a narrow region around the circle of radius $\langle m \rangle$ centered in the origin. A closer inspection to our data, reveals that such a motion has two main components. On one hand, $m(t)$ oscillates irregularly around its mean value, with a typical frequency $\Omega$ which is inversely proportional to $L$. On the other hand, the phase $\psi(t)$ performs a slower random motion whose displacement rapidly decreases with the energy. For instance, already below $e \simeq 0.3$ the phase changes of $M$ are hardly observable on the typical size and time scales of our simulations ($10^3 - 10^4$ time units).

These features of the motion of $M$ reflect into some distinctive properties of $S(0, \omega)$. More precisely, the oscillations of $m$ manifest themselves as a very sharp line at $\Omega$ (Fig. 1a), whereas the slower phase motion determines a low frequency ($\omega \ll \Omega$) component centered at $\omega = 0$ (Fig. 1b). The latter is naturally interpreted as a signature of phase diffusion, once we assume $\psi$ to be a Brownian variable with a diffusion time $D^{-1}$ much larger than the typical time scale of the motion of $m$. Accordingly, the spectrum is well fitted by a Lorentzian curve $C/(D^2 + \omega^2)$, which allows also to determine $D$. Furthermore, the relative weight of the diffusive component of $\langle |M(\omega)|^2 \rangle$ decreases upon decreasing $e$, in agreement with the qualitative observation that phase motion becomes less and less pronounced.

To further support this interpretation, we have computed the time evolution of the mean squared value $\sigma^2 = \langle (\psi - \psi_0)^2 \rangle$ for several lattice sizes. As shown in Fig. 2a, the data are consistent with a diffusive motion, i.e. $\sigma^2 = 2Dt$, for large enough $t$. We have also performed an independent measure of the diffusion constant based on Green-Kubo formula

$$D = \frac{1}{k_BT} \int_0^\infty \langle \dot{\psi}(t)\dot{\psi}(0) \rangle \, dt.$$  

(5)

Remarkably, the values computed using the three methods agree extremely well within the statistical accuracy (better than 15% in the worst case - see the inset of Fig. 2a).

In analogy with what happens for the static magnetization we expect the diffusion coefficient to approach zero on increasing the lattice size. Indeed, we found evidence that $D$ vanishes algebraically with a nontrivial exponent: a best fit to the data in the inset of Fig. 2 gives $D \propto L^{-1.6(3)}$ in the range $8 \leq L \leq 128$. Although we did not attempt to perform a systematic study, we have observed that a similar scaling holds also at lower energies. For instance, at $e = 0.70$ we found a slightly smaller exponent $\approx 1.5$ in the same range of sizes. Thus, we cannot rule out the possibility that such exponent depends on temperature in analogy with the one of finite-size magnetization.

The oscillations of $m$ are related to the spin-wave modes with the longest wavelength. We thus expect $\Omega$ to be proportional to $c/L$, where $c$ is the renormalized spin-wave velocity appearing in the effective dispersion relation

$$\omega^2 = 4c^2 \left[ \sin^2 \frac{q_x}{2} + \sin^2 \frac{q_y}{2} \right].$$  

(6)

Neglecting the contribution of vortices, $c$ is only determined by the anharmonic interaction among the spin-wave modes, thus leading to the estimate $-8c^2 \log c = k_BT$. The data
Fig. 1 – (a) Scaled high-frequency part of the spectrum $\langle |M(\omega)|^2 \rangle$ for $e = 0.992$ and $L = 64, 96, 128$. Each curve is an average of $\sim 10^3$ runs, each of $5 \times 10^3$ time units (sampling time 0.3). The thin dashed lines represent the power-laws $\omega^{-2}$ due to diffusion and the NF decay $\omega^{-2.75}$. (b) Low-frequency part of $\langle |M(\omega)|^2 \rangle$ obtained from longer runs ($3 \times 10^5$ time units) for $L = 8, 16, 32$ (from top to bottom). The spectra are not scaled and are in arbitrary units. Thin dashed lines are Lorentzian fits $C/(D^2 + \omega^2)$.

reported in Fig. 2 show that this results accurately describes the dependence of $\Omega$ on $T$ at least for low enough temperatures. Systematic deviation at larger temperature have of course to be expected due to the appearance of vortices. Indeed, it is usually believed [19] that their effect is to further diminish the spin-wave velocity, which is in qualitative agreement with our data.

Fig. 2 – (a) Mean squared displacement $\sigma^2 = \langle (\psi - \psi_0)^2 \rangle$ at $e = 0.992$ for $L = 16, 32, 64$ (from top to bottom). The inset shows the corresponding diffusion coefficient $D$ evaluated from a linear fit (circles), from Green-Kubo formula (squares) and from a Lorentzian fit of the low-frequency region of $\langle |M(\omega)|^2 \rangle$ (see Fig. 1b). (b) Scaled oscillation frequency $L\Omega$ versus the kinetic temperature for $L = 64, 128$ (circles and triangles respectively). The solid line is proportional to $c(T)$ (see text).
In order to better illustrate the new effects introduced by the finite lattice, we have evaluated the correlation \( \langle 3 \rangle \) in the low-temperature (spin-wave) region to lowest order (Gaussian theory). The resulting expression

\[
S(r,t) = \exp \left[ \frac{k_B T}{L^2} \sum_{q \neq 0} \frac{\cos \omega_q t e^{iq \cdot r} - 1}{\omega_q^2} \right]
\]  

(7)
is the lattice version of the formula obtained by NF in the continuum [15]. Their results can be summarized by saying that for \( \omega t \gg |r| \), \( S(r,t) \) should be independent of \( r \) and vanish algebraically in time as \( (\omega t)^{-\eta} \). We have evaluated numerically formula (7) by performing the sum over the discrete set of allowed \( q \)s for several values of \( r \). As a first check, we have found that \( S(r,t) \) is practically independent of \( r \) for \( r \ll L \). Therefore, we show in Fig. 3 the behavior of \( S(0,t) \) for several values of \( L \). We observe a dramatic difference with what expected from NF theory: (i) the power law decay is restricted to a small region of short times \( t \ll L \) and rather well-defined oscillations appear with typical period of order \( L \) at larger times; (ii) the correlation function does not vanish asymptotically, as it should be for a system with nonzero magnetization. The oscillating behavior of (5) is clearly due to the long-wavelength spin-waves and is therefore connected with the line structure around \( \Omega \) in Fig. 1a. Hence, this signals again that beyond the limit of validity of NF theory new effects due to the finite-size appear.

To summarize, in this Letter we have studied finite-size effects on the Hamiltonian dynamics of the magnetization vector \( M \) in the 2D XY model. We have investigated the consequences of the motion of the modulus and the phase of \( M \) on the behavior of the \( q = 0 \) structure factor. They amount to the appearance of a diffusive central component, which we associate to phase motion, and of a peak due to the oscillations of the modulus. The high frequency part is basically consistent with Nelson-Fisher theory [13]. Similar properties are observed for other types of dynamics [3], for which the shape of \( S(q,t) \) deviates from the one given by the Nelson-Fisher theory, exactly for the presence of a central peak. We conjecture that such features might be related to our results, and a more systematic comparison would be therefore desirable.

Furthermore, we have found a convincing evidence that the diffusion constant \( D \) vanishes algebraically with \( L \) with an exponent different from \( z = 1 \). If this would be confirmed for larger lattices, one should conclude that the correlation function does not exhibit a single scaling with \( L^z \), which in turn would imply a violation of the dynamic scaling hypothesis. This should be signalled by a bad superposition of the structure factor below \( \omega \sim D \) for different sizes. A direct test of this effect would however require simulations on much longer times. Since scaling violations indeed occur for coarsening phenomena [20], which are far off-equilibrium processes, it would interesting to investigate further this possibility also close to equilibrium.

***

We acknowledge useful discussions with H. Chaté, C. Godrèche, P. Simon. We thank P. C. W. Holdsworth for a careful reading of the manuscript. This work is supported by the INFM-PAIS project *Equilibrium and nonequilibrium dynamics in condensed matter*.

REFERENCES

[1] J. Tobochnik and G.V. Chester, *Phys. Rev. B*, 20 (1979) 3761.
Fig. 3 – Finite-size scaling of the correlation function $S(0,t)$, formula (7) for $k_B T = 0.05$ and $L = 128, 256, 512, 1024$. The scaling exponent is $\eta = k_B T / 2 \pi \approx 0.0079 \ldots$.

[2] R. Gupta and C.F. Baille, Phys. Rev. B, 45 (1992) 2883.
[3] R. Loft and T.A. DeGrand, Phys. Rev. B, 35 (1987) 8528.
[4] L.M. Jensen, B.J. Kim and P. Minnhagen, Phys. Rev. B, 61 (2000) 15412.
[5] H.G. Evertz and D.P. Landau, Phys. Rev. B, 54 (1996) 12302.
[6] J. Kogut and J. Polonyi, Nucl. Phys. B, 265 (1986) 313.
[7] D.E. Callaway and A. Rahman, Phys. Rev. Lett., 49 (1982) 613.
[8] X. Leoncini, A.D. Verga and S. Ruffo, Phys. Rev. E, 57 (1998) 6337.
[9] S.T. Bramwell et al., Phys. Rev. E, 63 (2001) 041106.
[10] S.T. Bramwell and P.C.W. Holdsworth, J. Phys. Condens. Matter, 5 (1993) L53.

It could be shown that (1) is obtained as the classical limit of a quantum Heisenberg Hamiltonian with an anisotropy term $\sum_r (S_z^r)^2$, using the representation introduced in J. Villain, J. Phys. (Paris), 35 (1974) 27.

[12] See Z. Gulácsi and M. Gulácsi, Adv. Phys., 47 (1998) 1 for a comprehensive review.
[13] P. Archambault, S.T. Bramwell and P.C.W. Holdsworth, J. Phys. A, 30 (1997) 8363.
[14] P.I. McLachlan and P. Atela, Nonlinearity, 5 (1992) 541.
[15] D.R. Nelson and D.S. Fisher, Phys. Rev. B, 16 (1977) 4945.
[16] For example, we checked that the data are compatible with the values 2.99 and 2.89 at $\epsilon = 0.05$ and 0.70 respectively. Notice that here the nonlinear corrections are basically irrelevant: the effective value of $\eta = k_B T / 2 \pi J_{eff}$ alters the value of the bare exponent by less than 1% in the latter case.
[17] W. Janke, Phys. Rev. B, 55 (1997) 3580.
[18] M. Cerrutti-Sola, C. Clementi and M. Pettini, Phys. Rev. E, 61 (2000) 5171.
[19] R. Coté and A. Griffin, Phys. Rev. B, 34 (1986) 6240.
[20] A.J. Bray, A.J. Briant and D.K. Jervis, Phys. Rev. Lett., 84 (2000) 1503.