Solitonic elliptical solutions in the classical XY model

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Abstract

The solitonic-like solutions predicted by the continuum semi-classical two–dimensional XY-model are investigated using canonical Monte Carlo simulation. In particular, we verify the existence of kink states, and study their degree of stability. These states, that were supposed to exist from approximate theories applied to the continuum limit of this model, are a new kind of solution of the XY model under external magnetic field. In the simulation several system sizes up to 100×100 spins were considered. The study of the static spin correlation between the initial and final configuration shows there exist a finite transition temperature T_c, which is independent of the system size. According to our simulation, at $T < T_c$ the kink state is stable, and the degree of stability increases with system size.

Key words: XY systems, kinks, Montecarlo simulation

1 Introduction

Among the classical spin systems, the XY model is one of the most relevant. It provides a prototype for systems which exhibit topological excitations and play a key role in the understanding on phase transitions, critical behavior, scaling, and universality [1,2]. In particular, the two dimensional XY model (2D-XY model) has been used to represent a wide variety of systems including superfluid films, Josephson-junction arrays, lipid layers, and others [3–5], in addition to the magnetic systems [6].

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The 2D-XY model may be viewed as a Heisenberg ferromagnetic with an easy-plane anisotropy, where the coupling between the z components of spins vanished. In general, the classical spins $\vec{S} = (S_x, S_y, S_z)$ interact only through the S_x, S_y components, and the third component, S_z, can be absent (called plane rotator model) or present (called XY model). Also, depending on the spatial coordinates, the XY model can be realized in one, two or three spatial dimensions. Interestingly, the plane rotator model and the $2D-XY$ model belong to the same universality class. The plane rotator model does not present any true long-range order, a consequence of the Mermin-Wagner theorem [7]. However, it presents a Kosterlitz-Thouless phase transition [8] at a finite temperature T_{KT}. Recent works suggest that the 2D-XY model also exhibit Kosterlitz-Thouless transition [9,10], very likely driven by a vortex-antivortex unbinding mechanism.

In this contribution we are interested in the 2D-XY model under in-plane magnetic field, widely used in superconductivity and magnetism [5]. The inclusion of an external in-plane magnetic field changes the behavior of the system, precluding any topological transition. Several types of solutions have been found in the 2D-XY under in-plane magnetic field, for instance spin waves, Kosterlitz–Thouless vortices [11], and spiral–antispiral pairs [12]. In addition to these well studied solutions, in Ref. [13], it was shown that in the continuum limit the 2D-XY Hamiltonian with an external magnetic field can be mapped onto an elliptic scale-invariant sine-Gordon equation [14] and exact solutions were obtained using Bäcklund transformations. These sine-Gordon solutions are solitonic excitations whose topology give evidence of kink like states. Our purpose is to examine the behavior of this kinks state, in particular, to study their degree of stability with respect to temperature or external magnetic field. This is done by means of computer simulation methods, namely MonteCarlo (MC) method [15]. A description of the model and the details of the computational procedures are given in Section 2. The results of the simulation are presented in Section 3 and the conclusions are drawn in Section 4.

2 Model and Computational Method

2.1 Theory

The Hamiltonian of the Heisenberg XY-model in two dimensions, with nearest neighbors ferromagnetic interactions reads as:

$$H = -J \sum_{i,j,\delta} \vec{S}_{i,j} \cdot \left[\vec{S}_{i+\delta,j} + \vec{S}_{i,j+\delta} \right] - \frac{h}{2} \sum_{i,j} S^x_{i,j} \quad (1)$$

where $J > 0$ is the ferromagnetic exchange interaction parameter, $h = g\mu_B H$ with H the external magnetic field applied along the $x-$axis and $\delta = d$ (d lattice parameter). g is the $g-$factor and μ_B is the Bohr magneton.

In the continuum limit, using raising and lowering spin operators and to second order in δ this Hamiltonian takes the form

$$H = -\frac{1}{2}J \int\int dx\, dy \Big[\frac{1}{2}\Big\{S^{+}(x,y)\nabla^2 S^{-}(x,y) + S^{-}(x,y)\nabla^2 S^{+}(x,y)\Big\} + S^{z}(x,y)\nabla^2 S^{z}(x,y)\Big] - \frac{h}{2}\int\int dx\, dy \Big(S^{+}(x,y) + S^{-}(x,y)\Big) \quad (2)$$

Using the Schwinger [16] transformation and the semi-classical approximation that the spins can be continuously projected along the quantization axis it was demonstrated [13], in the coherent state formalism [17], that the system obeys the following time independent scale-invariant elliptic sine-Gordon equation:

$$\nabla^2 \Phi(\vec{r}) = m^2 \sin(\Phi(\vec{r})) \ , \quad (3)$$

where $\Phi(\vec{r})$ is the angle that the spin in $\vec{r}$ forms with respect to an external field H and $m^2 \equiv 8g\mu_B H/3J$. This equation is scale invariant since the magnitude m can be absorbed in a variation of the length scale.

By using a Bäcklung transformation [18] we found in Ref. [13] that a solution to that equation is a plane static soliton

$$\Phi(\vec{r}) = 4\ \arctan(A \exp(\vec{r}\cdot\vec{\alpha})) \ , \quad (4)$$

where A is a constant, $\vec{\alpha} \equiv \cos(\rho)\cdot\hat{x} + \sin(\rho)\cdot\hat{y}$ and ρ a Bäcklung parameter. Figure 1 displays this kink state for $A = 1$ and $\rho = \pi/8$. Notice that this result constitute another types of solution of the 2D-XY model, different from the well-known metastable vortex-antivortex pair of the Kosterlitz-Thouless theory [19,20].

2.2 Simulation

We study the kink-like solutions by means of a MC simulation. In order to do that, we consider a classical XY model with two spin component in two dimensions (plane rotator model) under an external magnetic field, using as a initial configuration the kink solution given by Equation (4).

The Hamiltonian reads as

$$H = -J \sum_{i,j,\delta} \hat{s}_{i,j} \cdot [\hat{s}_{i+\delta,j} + \hat{s}_{i,j+\delta}] - h \sum_{i,j} s^x_{i,j} \ , \tag{5}$$

where $\hat{s}_{i,j}$ are classical vectors of unit length taken from the continuous spin variable $\vec{S} = S\hat{s}$, with $J = \tilde{J}S^2$, and $h = S\tilde{h}/2$ [21].

The properties of the system with respect to temperature were obtained by using standard Metropolis Monte Carlo method [15]. We consider three different system sizes, 15×15, 25×25, and 100×100. For each system, the initial configuration is the one corresponding to Figure 1, and the temperature goes from 0 to 5 k_B/J, at intervals of 0.1 k_B/J for low temperatures, and 0.5 k_B/J for high temperatures. After equilibration, 2×10^3 MC steps per spin at each temperature were performed. This number of steps was chosen after performing longer run for some temperatures without significant differences. In all simulations the external magnetic field correspond to $h = 0.1\ J$.

The analysis of the result was done by means of the correlation with respect to initial configuration,

$$C = \langle s^x_i(0) s^x_i(n) + s^y_i(0) s^y_i(n) \rangle$$

where $s^x_i(0)$ and $s^y_i(0)$ are the components of spin i of the initial configuration and $s^x_i(n)$ and $s^y_i(n)$ correspond to the components of spin i of the configuration n. The average $\langle \ldots \rangle$ is done over all n uncorrelated configuration of each run.

3 Results

Figure 2 shows a typical final spin configuration at $T = 0.01\ k_B/J$. We can see that the main features of the kink persist, presenting only little differences with respect to the original configuration. Among them are the widening of the kink as well as the formation of kind of vortices at each end. This configuration does not change when we increase the number of MC steps.

When the temperature increase, the kink state get disorder, but it is still present, as can be seen in Figure 3, where it is shown a typical final spin configuration at $T = 0.4\ k_B/J$. Notice that in this case the kink is even wider than in the former case, and it is clearly distinguishable the pair vortex-antivortex at each end of the kink. These vortices can be considered as a resemblance of the Kosterlitz-Thouless vortices solution of the sine-Gordon equation, and also are present in the case of the spiral solutions discussed in Ref. [12].

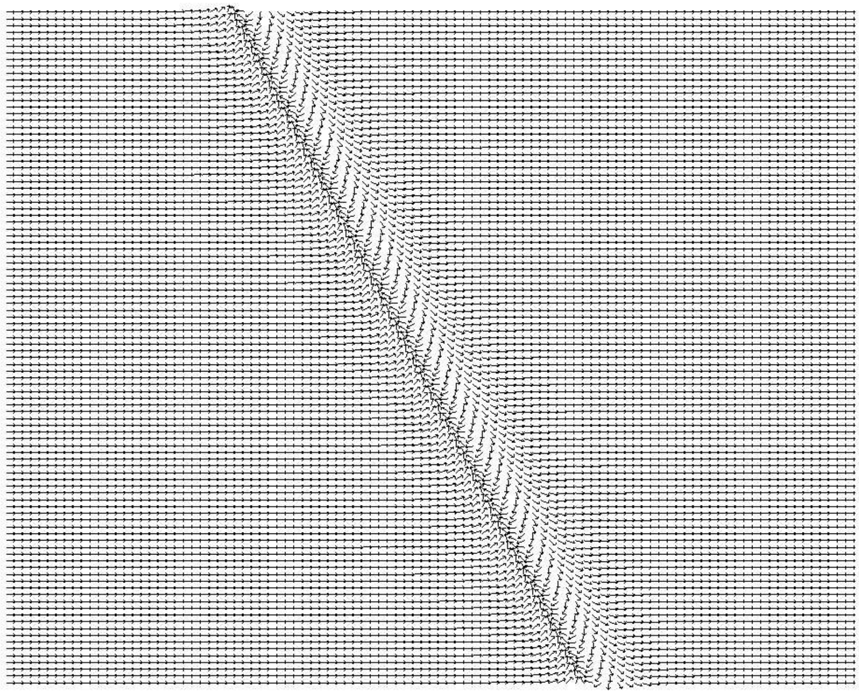

Fig. 1. Initial configuration in the case of a lattice of 100×100 spins. This is the kink state corresponding to Equation (1) with $A = 1$ and $\rho = \pi/8$.

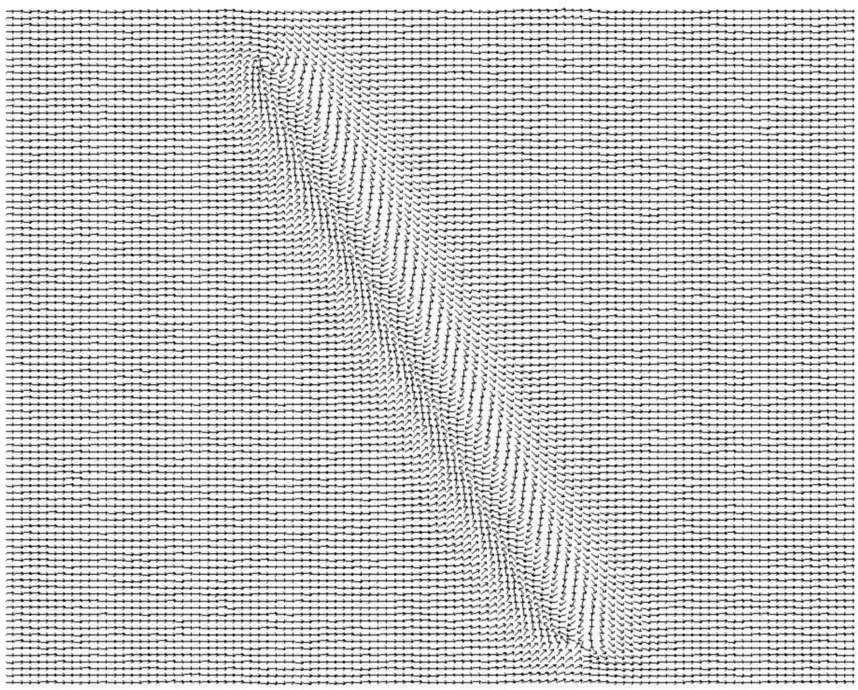

Fig. 2. Spin configuration at $T = 0.01\ k_B/J$ and $h = 0.1\ J$.

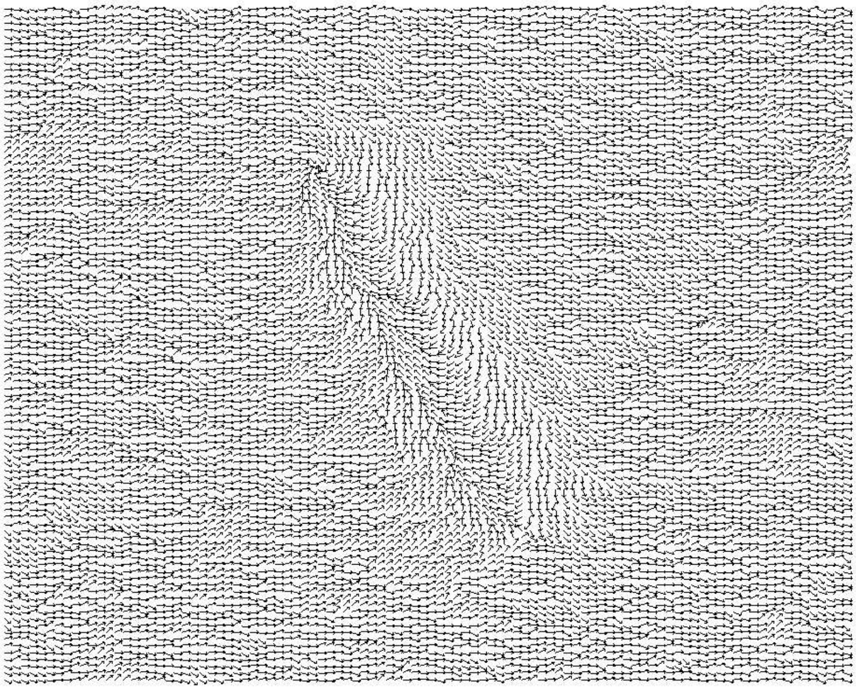

Fig. 3. Spin configuration at $T = 0.4\ k_B/J$ and $h = 0.1\ J$.

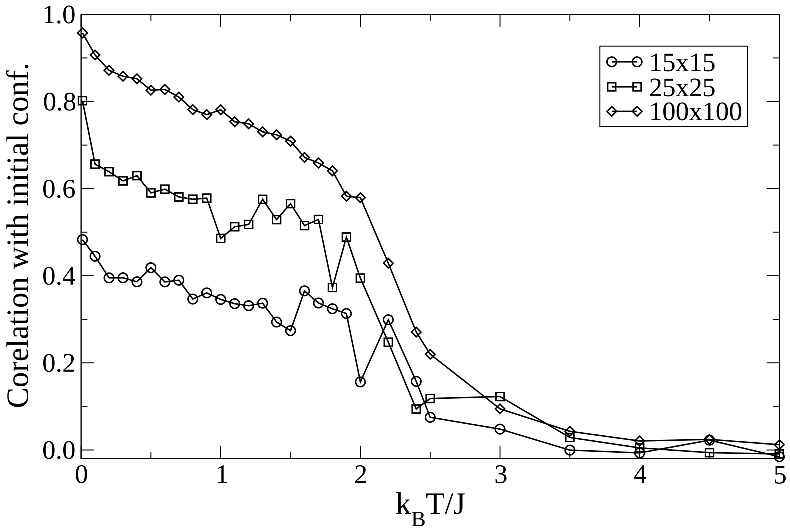

Fig. 4. Correlation with respect to the initial configuration, for sizes 15×15, 25×25, and 100×100 spins.

The kink state persist up to certain finite transition temperature T_c, and above T_c it disappear. Figure 4 shows how his process occurs. For low temperatures, the correlation between the initial and the final configuration is significant, meaning that the kink state is observable. At high temperature the correlation goes to zero, that is, the kink disappear. The temperature at which this transition happen can be estimate around $2.5\ k_B/J$. Notice that T_c is almost the same for the three different sizes of the system. Also, it is interesting to note that for the same temperature, the larger the system the bigger the correlation, a trend that is expected because the kink solution of Equation (5) was obtained in the continuum semiclassical limit. This is a proof of the internal consistency of our simulation.

4 Concluding remarks

We have investigated the behavior with respect to temperature, under a fix external magnetic field, of solitonic solutions, so-called kink states, predicted by the continuum semi-classical XY-model. By means of MC numerical simulation we verify the existence of these solutions also in the discrete model, for systems up to 100×100 spins.

The correlation of these kink states with respect to the initial configuration shows a strong dependence with the temperature making evident the existence of a finite transition temperature T_c. Moreover, for our particular set of parameter we were able to estimate this temperature around 2.5 k_B/J. Also, by long MC run, we check for some cases that below T_c the kink state are stable. Finally, we notice that the final MC states are much more correlated with the initial configuration state when the system includes a larger number of spin sites, consistent to fact that increasing the size of the system (number of spins) improves the validity of the analytical solutions of the continuum semi-classical limit. However the temperature at which the correlation vanishes is independent system size.

Acknowledgments

G. G. is supported by FONDECYT (Chile) under Grant No. 1030063 and *Núcleo Milenio Física de la Materia Condensada* P02-054-F.

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[21] According this definition, $\tilde{J}$ and $\tilde{h}$ correspond to J and h of the original quantum hamiltonian of Equation (1), respectively.