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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 exists a finite transition temperature T_c. According to our simulation, at $T < T_c$ the kink state is stable, and the degree of stability increases with system size.

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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 plays a key role in the understanding on phase transitions, critical behavior, scaling, and universality [1]. 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, in addition to the magnetic systems [2].

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 $\boldsymbol{S} = (S_x, S_y, S_z)$ interact only through the S_x, S_y components, and the third component, S_z, may 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 both belong to the same universality class.

In this contribution, we are interested in the 2D-XY-model under in-plane magnetic field. 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 [3], and spiral–antispiral pairs [4]. In addition to these well studied solutions, it was shown in Ref. [5] 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 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 these kink states, in particular, to study their degree of stability with respect to temperature or external magnetic field by means of computer simulation methods, namely Monte Carlo (MC) method [6].

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

$$H = -J \sum_{i,j,\delta} \boldsymbol{S}_{i,j} \cdot [\boldsymbol{S}_{i+\delta,j} + \boldsymbol{S}_{i,j+\delta}] - \frac{h}{2} \sum_{i,j} S^x_{i,j}, \tag{1}$$

where $J > 0$ is the ferromagnetic exchange interaction parameter, $h = g\mu_{\mathrm{B}} H$ with H the external magnetic field

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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

$$H = -\frac{1}{2}J\int\int \mathrm{d}x\,\mathrm{d}y\left[\frac{1}{2}\{S^+(x,y)\nabla^2 S^-(x,y) + S^-(x,y)\nabla^2 S^+(x,y)\} + S^z(x,y)\nabla^2 S^z(x,y)\right] - \frac{h}{2}\int\int \mathrm{d}x\,\mathrm{d}y(S^+(x,y) + S^-(x,y)). \quad (2)$$

Using the Schwinger transformation and the semi-classical approximation in the coherent state formalism, it can be demonstrated [5] that the system obeys the following time independent scale-invariant elliptic sine-Gordon equation:

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

where $\Phi(\mathbf{r})$ is the angle that the spin in $\mathbf{r}$ 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, it is found [5] that sine-Gordon equation has by solution a plane static soliton

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

where A is a constant, $\boldsymbol{\alpha} \equiv \cos(\rho)\cdot\hat{x} + \sin(\rho)\cdot\hat{y}$ and ρ, a Bäcklung parameter. Fig. 1 displays this kink state for $A = 1$ and $\rho = \pi/8$.

To study these kink-like solutions by means of a MC simulation, we consider a classical XY-model with two spin component in two dimensions (plane rotator model) under an external magnetic field. The Hamiltonian reads

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

where $\hat{s}_{i,j}$ are classical vectors of unit length taken from the continuous spin variable $\mathbf{S} = S\hat{s}$, with $J = \tilde{J}S^2$, and $h = S\tilde{h}/2$ [7].

The properties of the system with respect to the temperature were obtained by using standard Metropolis Monte Carlo method [6]. We consider three different system sizes: 15×15, 25×25 and 100×100. For each system, the initial configuration is the one corresponding to Fig. 1, and the temperature goes up to $5\,\mathrm{J/k_B}$, at intervals of $0.1\,\mathrm{J/k_B}$ for low temperatures, and $0.5\,\mathrm{J/k_B}$ for high temperatures. After thermalization, 2×10^3 MC steps per spin at each temperature were performed. This number of steps was chosen after performing longer runs for some temperatures without significant differences. In all simulations, the external magnetic field corresponds to $h = 0.1\,\mathrm{J}$.

The analysis of the result was done by means of the correlation

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

with respect to initial configuration, where $s^x_i(0)$ and $s^y_i(0)$ are the components of ith spin of the initial configuration and $s^x_i(n)$ and $s^y_i(n)$ are those corresponding to the components of ith spin of the configuration n. The average $\langle\cdots\rangle$ is done over all n uncorrelated configuration of each run.

Fig. 2 shows a typical final spin configuration at $T = 0.01\,\mathrm{J/k_B}$. We observe 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 vortices at each end. This configuration does not change when we increase the number of MC steps.

When the temperature increases, the kink state get disorder, but it is still present, as can be seen in Fig. 3, where it is shown a typical final spin configuration at $T = 0.4\,\mathrm{J/k_B}$. Note that in this case the kink is even wider than in the former case, and it is clearly distinguishable the

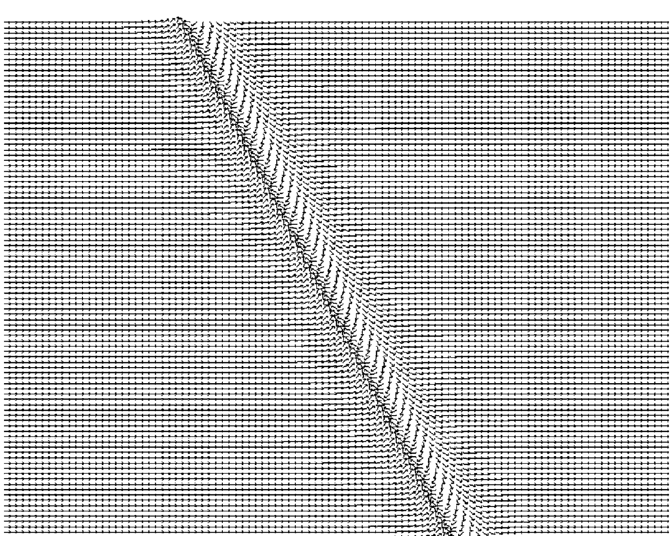

Fig. 1. Initial configuration in the case of a lattice of 100×100 spins. This is the kink state corresponding to Eq. (1) with $A = 1$ and $\rho = \pi/8$.

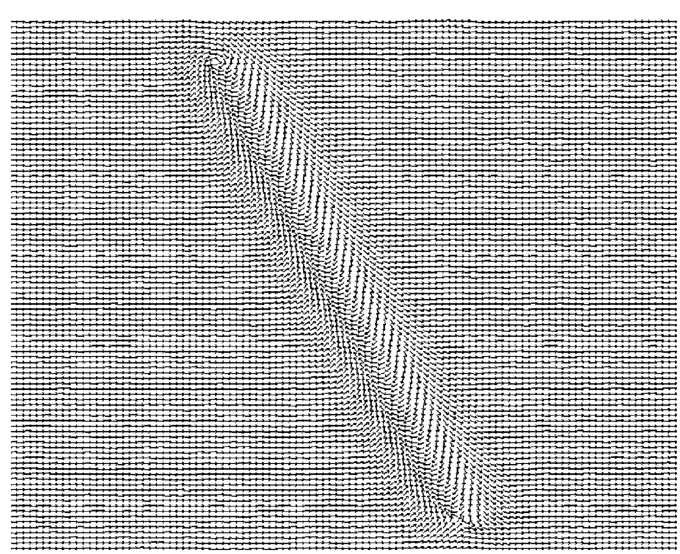

Fig. 2. Spin configuration at $T = 0.01\,\mathrm{J/k_B}$ and $h = 0.1\,\mathrm{J}$.

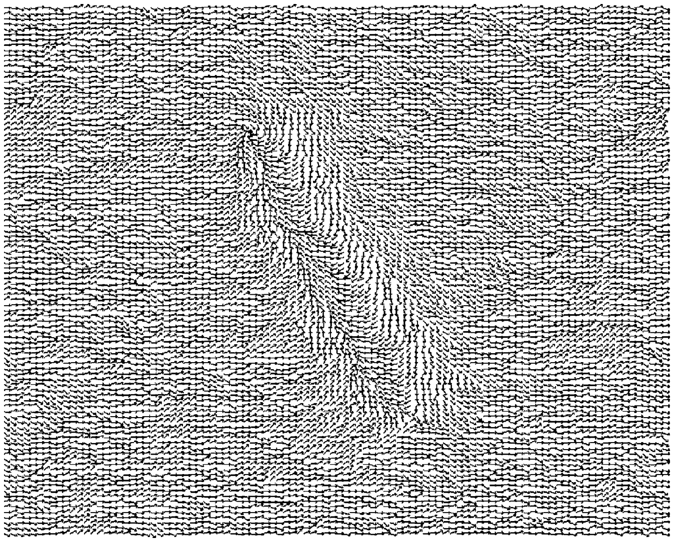

Fig. 3. Spin configuration at $T = 0.4\,\mathrm{J/k_B}$ and $h = 0.1\,\mathrm{J}$.

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 [8], and also are present in the case of the spiral solutions discussed in Ref. [4].

The kink state persists up to certain finite transition temperature T_c and, above T_c, it disappears. Fig. 4 shows how this 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 disappears. The temperature at which this transition happens can be estimated around $2.5\,\mathrm{J/k_B}$. Note 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 Eq. (5) was obtained in the continuum semiclassical limit. This is a proof of the internal consistency of our simulation.

In summary, we have investigated the behavior with respect to temperature, under a fixed external magnetic field, of solitonic solutions, the so-called kink states, predicted by the continuum semi-classical XY-model. 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

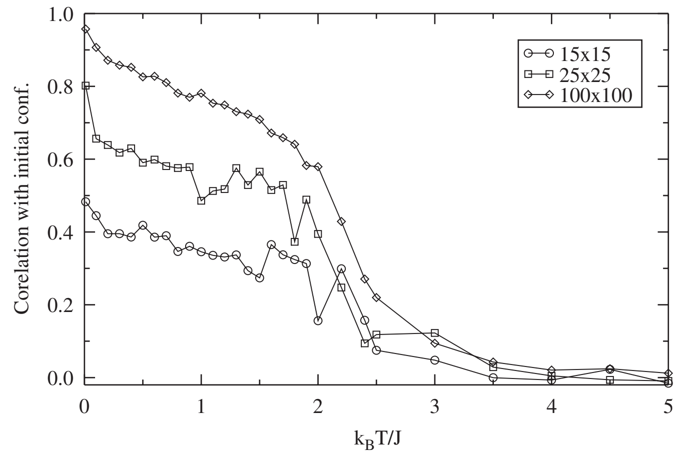

Fig. 4. Correlation with respect to the initial configuration, for sizes 15×15, 25×25 and 100×100 spins.

parameter we were able to estimate this temperature around $2.5\,\mathrm{J/k_B}$. Also, by long MC run, we checked for some cases that below T_c the kink states are stable. Finally, we conclude 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 with the fact that increasing the size of the system (number of spins) this improves the validity of the analytical solutions of the continuum semi-classical limit.

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

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