MONTE CARLO STUDY OF THE XY-MODEL ON SIERPIŃSKI CARPET

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We have performed a Monte Carlo study of the classical XY-model on a Sierpiński carpet, which is a planar fractal structure with infinite order of ramification and fractal dimension 1.8928. We employed the Wolff cluster algorithm in our simulations and our results, in particular those for the susceptibility and the helicity modulus, indicate the absence of finite-temperature Berezinskii-Kosterlitz-Thouless (BKT) transition in this system.

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1. Introduction

In a translationally invariant system the critical behavior is determined by its universality class which depends on the symmetry of the Hamiltonian, the spatial dimension of the system, and the range of forces between the particles. Systems with fractal structure lack translational invariance but are scale invariant and have additional topological features, such as the fractal dimension, the order of ramification, the connectivity, and the lacunarity, which could influence the phase transition in these systems (see References 1–6). Much is known about the phase transitions for the discrete-symmetry Ising model on various fractal structures (Refs. 1, 2, 3, 4, 6) but very little is known about the continuous-symmetry models, such as the classical XY-model, on fractals. In a recent work we used the Metropolis Monte Carlo (MC) method to examine the classical XY-model on two fractal structures with finite orders of ramification, Sierpiński gasket and Sierpiński pyramid, and found no phase transition at any finite temperature. These results were analogous to what was obtained previously for the Ising model on finitely ramified frac-
tals using the renormalization group method. The order of ramification \( R \) at a point \( P \) of a structure is defined as the number of bonds which must be cut in order to isolate an \( \text{arbitrarily large} \) bounded set of points connected to \( P \) (e.g. the regular periodic lattices have \( R = \infty \)). In systems with finite \( R \) the thermal fluctuations at any finite temperature destroy long-range order (no finite-temperature continuous phase transition), as well as quasi-long-range order (no finite-temperature Berezinskii-Kosterlitz-Thouless (BKT) transition). These conclusions hold regardless of the symmetry of the microscopic Hamiltonian (i.e. whether it has a discrete \( Z_2 \) symmetry (Ising) or a continuous \( O(2) \) symmetry (XY)).

For discrete-symmetry spin models on infinitely ramified Sierpiński carpets, Gefen, Aharony, and Mandelbrot\(^4\) found phase transitions at finite temperature (see also the work of Wu and Hu\(^9\) where some of the recursion relations in Ref.\(^4\) have been corrected). Moreover, using a correspondence between a resistor network connecting the sites of a given lattice and the low-temperature properties of \( n \)-component spin models, with \( n \geq 2 \), on the same lattice\(^10\) they argued that there is no long-range order at any finite temperature if the fractal dimension \( D < 2 \), even when \( R = \infty \). They conjectured that the reason for the absence of the long-range order is that for \( O(n) \) spin models the lower critical Euclidean dimension is \( d = 2 \), and for a fractal in \( d \) dimensions one has \( D \leq d \).

Here we present a Monte Carlo study of the classical XY-model on a two-dimensional Sierpiński carpet depicted in Figure\(^1\) described by the Hamiltonian

\[
H = -J \sum_{\langle i, j \rangle} \cos(\theta_i - \theta_j),
\]

(1)

where \( 0 \leq \theta_i < 2\pi \) is the angle variable on site \( i \), \( \langle i, j \rangle \) denotes the nearest neighbors, and \( J > 0 \) is the coupling constant. In the notation of Gefen \textit{et al.}\(^4\), the

Fig. 1. The first step in creating Sierpiński carpets with \( b=3 \) and \( l=1 \).
Sierpiński carpet studied here was generated by starting from the first order carpet consisting of $b \times b$ sites, with $b = 3$, from which $l^2$ centrally located sites, $l = 1$, were removed. Then the carpet of order $m$ was obtained from the carpet of order $m-1$ by translating it with seven translation vectors as illustrated in Figure 1. Since the outer edge of the $m$th order carpet is identical to the outer edge of a $3^m \times 3^m$ square lattice, it is immediately clear that $R = \infty$ for the Sierpiński carpets. The fractal dimension of our carpet is $D = \frac{\ln(b^2 - l^2)}{\ln b} = \frac{\ln 8}{\ln 3} = 1.8928$, and its connectivity $Q$, which is defined as the smallest of the fractal dimensions of the boundaries of the bounded subsets of the carpet, is $Q = \frac{\ln(b - l)}{\ln b} = \frac{\ln 2}{\ln 3} = 0.6309$, see Ref. [4]. The defining property of all fractals is that they are scale invariant but not translationally invariant. The lacunarity $L$ of a fractal measures its deviation from translational symmetry and the amount of inhomogeneity. Using an approximation for $L$ proposed by Gefen et al. we find $L = 0.0988$. This is much smaller than the values for two $b = 7$ and $l = 3$ Sierpiński carpets considered in Ref. [4] (for translationally invariant systems $L = 1$).

We computed the heat capacity, the susceptibility and the helicity modulus for Sierpiński carpets of orders $m = 2$–5 (the number of sites in the carpet of order $m$ is $N = 8^m$, and we take the smallest $m = 1$ carpet to have lattice spacing equal to one). The dependence of the helicity modulus on the size of the carpet, and on the boundary conditions, clearly indicates that in the thermodynamic limit there is no BKT transition at any finite temperature.

The rest of the paper is organized as follows. In Section 2 we outline the numerical procedure used in calculations and then we present and discuss our numerical results in Section 3. Finally, in Section 4 we give a concise overview of our findings.

2. Calculation

We have used Monte Carlo simulations based on the Wolff cluster algorithm which avoids the critical slowing down associated with a diverging correlation length in the vicinity of a phase transition. One MC step involved generating a cluster of correlated spins as described in Ref. [13], and then flipping those spins about the randomly chosen reflection axis for that step. For each temperature we discarded the first 120,000 MC steps, which allowed for the system to equilibrate. We then generated an additional seven links, each of 120,000 MC steps, and the final configuration after computing these seven links was used as the initial configuration for the next higher temperature. We estimated the error in our calculations by breaking up each of the seven links into six blocks of 20,000 MC steps, then calculating the average values for each of the 42 blocks and finally taking the standard deviation $\sigma$ of these 42 average values as an estimate of the error.

Since the characteristic feature of fractals is scale invariance (and not translational invariance), we could not employ the periodic boundary conditions. Instead, we used just two types of boundary conditions: open (or free) and closed. For the closed boundary condition, each of the four outer corners of an $m$th order carpet is
coupled to the closest two of the remaining three outer corners, while in the open boundary condition none of the outer corners are coupled to each other. The heat capacity per site $C$, and the linear susceptibility per site $\chi$, were computed in a standard way using the fluctuation theorems, as in our previous Monte Carlo studies\cite{7,8}. From the fluctuations in energy, $C$ was calculated as follows:

$$C = \frac{1}{N} \frac{1}{k_B T^2} \left\langle H^2 \right\rangle - \left\langle H \right\rangle^2,$$

and $\chi$ was computed in a similar manner, using the fluctuations in magnetization per site $\langle m \rangle$:

$$\chi = \frac{1}{k_B T} \left\langle m^2 \right\rangle - \langle m \rangle^2.$$

In equations (2) and (3) $k_B$ is the Boltzmann constant, $T$ is the absolute temperature, and $\langle \cdots \rangle$ denotes the MC average. To calculate the helicity modulus $\gamma$ we used the same procedure as in our earlier work, which was first proposed by Ebner and Stroud\cite{14}. In this procedure, the XY Hamiltonian (equation (1)) is thought of as describing a set of Josephson-coupled superconducting grains in zero magnetic field. The variable $\theta_i$, which gives the direction of spin on the lattice site $i$, becomes the phase of the superconducting order parameter for that site. An applied uniform vector potential $A$ causes a shift in the phase difference $\theta_i - \theta_j$ of the XY Hamiltonian by the amount $2\pi A \cdot (r_j - r_i) / \Phi_0$, with $r_i$ the position vector of site $i$, and $\Phi_0 = hc/2e$ the flux quantum. The helicity modulus $\gamma$ is given by the second derivative of the Helmholtz free energy per site with respect to uniform $A$, at $A = 0$. One finds

$$\gamma = \frac{1}{N} \left[ \left\langle \left( \frac{\partial^2 H}{\partial A^2} \right)_{A=0} \right\rangle - \frac{1}{k_B T} \left\langle \left( \frac{\partial H}{\partial A} \right)^2 \right\rangle_{A=0} + \frac{1}{k_B T} \left\langle \left( \frac{\partial H}{\partial A} \right)_{A=0} \right\rangle^2 \right],$$

with $H$ the phase-shifted XY Hamiltonian. By applying a uniform vector potential along one of the edges of the Sierpinski carpet (e.g. $A$ along the $x$-axis), only nearest neighbors whose $x$-coordinates differ by $\pm 1$ (the smallest lattice spacing) will contribute to $\gamma$, as a consequence of the square symmetry of the carpet.

3. Results and Discussion

Our results for the heat capacity per site for both the open and closed boundary conditions are presented in Figure 2. The increasing size of the error bars with increasing temperature is a consequence of the fact that the size of the clusters of correlated spins in the Wolff algorithm decreases with increasing temperature. Hence, a larger number of Monte Carlo steps is required at higher temperatures. The results shown in Figures 2, 4, and 6 at $k_B T/J \geq 0.55$ were obtained by using 600,000 MC steps per link instead of 120,000 MC steps per link, which reduced the size of the error bars by about a factor of two.
We have examined the dependence of the maximum in the specific heat $C_{\text{max}}$ on the system size, Figure 3. The data on $C_{\text{max}}$ obtained with open boundary condition were fitted with the formula

$$C_{\text{max}}(N) = C^\infty + \frac{Q}{(\ln N)^a},$$

where $N$ is the number of sites in the carpet. We obtained $C^\infty = 1.134$, $Q = -0.858$ and $a = 0.86$ with the $\chi^2$ of the fit equal to $5.938 \times 10^{-6}$. The maximum in the specific heat $C$ saturates with increasing system size. The classical XY-model on two-dimensional regular lattices displays BKT transition from quasi-long-range order (order parameter correlation function decays algebraically) to disordered phase (order parameter correlation function decays exponentially). The transition results from unbinding of topological defects (vortices and antivortices) and the specific heat has an unobservable essential singularity at the transition temperature $T_c$. The maximum in heat capacity is above the transition temperature and is caused by unbinding of vortex clusters with increasing temperature above $T_c$. As a result
it saturates with increasing system size in Monte Carlo simulations. While the saturation in $C$ with increasing system size is not sufficient to prove the existence of BKT transition at finite temperature, it is a necessary consequence if this transition does take place in an infinite system.

![Graph](image)

**Fig. 3.** The maximum in the specific heat as a function of the system size for closed boundary condition (filled circles) and open boundary condition (open circles). The solid line is a fit to the results with open boundary condition obtained with equation (5).

We would like to point out that while in MC simulations of the classical XY-model on the square lattice (see also Figure 2 in Ref. 7) the temperature $T^*$ at which the specific heat has maximum $C^\text{max}$ slowly decreases with increasing system size, we find the opposite trend for the Sierpiński carpet. For the carpets with $N = 64, 512, 4096,$ and $32768$ we obtained $T^*/J = 0.6, 0.7, 0.75,$ and $0.75,$ respectively, with open boundary condition, and $T^*/J = 0.7, 0.7, 0.7,$ and $0.75,$ respectively, with closed boundary condition.

Our results for the susceptibility are given in Figure 4. The trend in the change of shape in $\chi$ with increasing system size is similar to what we obtained for the classical XY-model on the square lattice; the peaks in $\chi$ increase in height and move to lower temperatures with increasing system size. We saw this behavior in both the Sierpiński gasket and Sierpiński pyramid, but with a more substantial shift in the peak position with increasing system size. For these finitely ramified fractals, we concluded that in the thermodynamic limit, there was no finite-temperature transition. For the BKT transition, Kosterlitz predicted that above the transition
temperature $T_c$ the susceptibility diverges as $\chi \sim \exp[(2-\eta)b(T/T_c-1)^{-\nu}]$, with $\eta = 0.25$, $b \approx 1.5$, and $\nu = 0.5$, and is infinite below $T_c$. For finite systems one gets finite peaks in $\chi$ above $T_c$. In Figure 5 we show how the temperature $T_\chi$ corresponding to

$$T_\chi(N) = R + S(\ln N)^b$$

(6)

gave $R = 0.85$, $S = -0.048$, and $b = 1$ with the $\chi^2$ of the fit equal to $1.6 \times 10^{-9}$ (solid line in Figure 5). This would imply that $T_\chi$ would become 0 for $N = 4.7 \times 10^7$, which practically corresponds to the thermodynamic limit. We also fitted the data for $T_\chi$ according to

$$T_\chi(N) = U + \frac{W}{N^c}$$

(7)
(i.e. an exponential fit in ln \(N\)) and obtained \(U = -0.238\), \(W = 1.17\), and \(c = 0.0646\) with the \(\chi^2\) of the fit equal to \(1.9 \times 10^{-4}\) (dashed line in Figure 5). The negative value of \(U\) implies that \(T_\chi\) is not positive in the thermodynamic limit, i.e. that there is no finite-temperature BKT transition in the thermodynamic limit (equation (7) gives \(T_\chi = 0\) for \(N = 5.1 \times 10^{10}\), which again corresponds to the thermodynamic limit).

![Image](image_url)

**Fig. 5.** The dependence of the temperature where the susceptibility attains the maximum on the system size. The solid line gives a fit to the data according to equation (6) and the dashed line gives a fit according to equation (7).

The best indicator of the BKT transition in the numerical work is the temperature dependence of the helicity modulus \(\gamma\) which measures the stiffness of the angles \(\{\theta_i\}\) with respect to a twist at the boundary of the system. At zero temperature, when the angles are all aligned, the value of \(\gamma\) is finite, and at sufficiently high temperature, when the system is in the disordered paramagnetic phase, \(\gamma = 0\). In the case of the classical XY-model on three-dimensional regular lattices \(\gamma(T)\) decreases continuously with increasing temperature and just below the transition temperature \(T_c\) it obeys a power law \(\gamma(T) \propto |T - T_c|^v\) (Ref. 19). In two dimensions Nelson and Kosterlitz 20 predicted a discontinuous jump in \(\gamma\) at the BKT transition temperature \(T_c\) with a universal value \(\gamma(T_c)/T_c = 2/\pi\). For a finite system the jump in \(\gamma\) is replaced by continuous decrease with increasing \(T\), which becomes steeper near \(T_c\) as the system size increases.

Our results for \(\gamma\) are shown in Figure 6 for the open and closed boundary con-
ditions. The two important similarities between these results and the ones obtained for fractals with finite order of ramification \cite{7,8} are: (1) In both classes of fractals, the open boundary condition led to $\gamma = 0$, within the error bars, at finite temperatures.

Fig. 6. Calculated helicity modulus as a function of temperature and system size with both types of boundary conditions.

(2) In each case, the closed boundary condition led to finite low-temperature values of $\gamma$ which decrease with increasing system size. Moreover, the onset of the downturn in $\gamma$, which is in the vicinity of the universal $2/\pi$-line, moves to the lower temperatures with increasing system size. In the case of the $XY$-model on regular lattices (see Figure 4 in Ref. \cite{7} for the results obtained on the square lattices), low-temperature values of the helicity modulus do not depend on the system size. Furthermore, the onset of the downturn in $\gamma$ is not size dependent, and it occurs at the same temperature for each square lattice considered.

In Figure 7 we show how the low-temperature value of the helicity modulus obtained with closed boundary condition depends on the system size. The data were fitted according to
\[ \gamma_{\text{max}}(N) = X + \frac{Y}{(\ln N)^f} \]  

(8)

with \(X = 2.67 \times 10^{-9}\), \(Y = 1.16\), and \(f = 0.723\), and the \(\chi^2\) of the fit was \(8.8 \times 10^{-20}\). A fit where \(X\) was set equal to 0 gave the same values for \(Y\) and \(f\) with the \(\chi^2\) of \(4 \times 10^{-4}\). Clearly the low-temperature value of the helicity modulus obtained with closed boundary condition goes to zero in the thermodynamic limit. As a result, we conclude that the Monte Carlo simulation results for the classical XY-model on the Sierpiński carpet with \(b = 3\) and \(l = 1\) indicate the absence of finite temperature BKT transition in the thermodynamic limit.

4. Conclusions

We have performed an extensive Monte Carlo study of the classical XY-model on the Sierpiński carpet with \(b = 3\) and \(l = 1\) which has infinite order of ramification \(R\), fractal dimension \(D = 1.8928\), connectivity \(Q = 0.6309\), and lacunarity \(L = 0.0988\). Our results for the helicity modulus obtained with closed boundary conditions for a given order carpet exhibit temperature dependence similar to what we expect in square lattices undergoing BKT transition: a continuous drop near the \(2/\pi\) line. However, the dependence of the low-temperature values of the helicity
modulus on the system size, as well as on the boundary conditions, implies that there is no finite-temperature BKT transition in this system in the thermodynamic limit. The numerical results for the dependence of the temperature where the susceptibility attains the maximum value on the system size are completely consistent with this conclusion. The absence of finite-temperature BKT transition in this infinitely ramified planar fractal is likely related to the fact that its fractal dimension $D$ is less than 2. A further analysis along the lines of Ref. 5 for finitely ramified planar Sierpiński gasket would be required to clarify this.

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