Absence of phase transition in the XY-model on Menger sponge

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Abstract

We have performed a Monte Carlo study of the classical XY-model on a Menger sponge with the Wolff cluster algorithm (U. Wolff, 1989). The Menger sponge is a fractal object with infinite order of ramification and fractal dimension \( D = \frac{\log(20)}{\log(3)} = 2.7268 \). From the dependence of the helicity modulus on system size and on boundary conditions, we conclude that there is no phase transition in the system at any finite temperature.

Keywords: XY-model, fractal, Menger sponge, Monte Carlo simulations.

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1. Introduction

In our previous Monte Carlo (MC) studies of the classical XY-model on Sierpiński gasket with $D = 1.585$ [1], and on Sierpiński pyramid with fractal dimension $D = 2$ [2], we observed the absence of any finite temperature phase transition. These fractal lattices both have a finite minimum order of ramification, $R_{\text{min}}$. The Sierpiński pyramid has $R_{\text{min}} = 4$, while Sierpiński gasket has $R_{\text{min}} = 3$. The order of ramification $R$ at a point $P$ of a lattice is the number of significant bonds one must break to isolate an arbitrarily large cluster of points surrounding $P$ from the rest of the lattice. Regular, translationally invariant systems, which fill space uniformly, have infinite order of ramification. In contrast, fractals, which are by definition scale invariant but not translationally invariant, do not fill space uniformly and may have a finite order of ramification. In fractals with finite $R$, any cluster of points can be cut off from the rest of the structure by breaking only a finite number of bonds. Consequently, thermal fluctuations in these systems are sufficient to destroy the long range order associated with continuous phase transitions, as well as the quasi-long range order associated with the Berezinskii-Kosterlitz-Thouless (BKT) transition, exhibited by the XY-model in translationally invariant two-dimensional systems. This behavior is independent of the microscopic model and has been observed for spin models with discrete symmetry (Ising model, discrete $Z_2$ symmetry) [3, 4, 5, 6] as well as models with continuous symmetry (XY-model, continuous $O(2)$ symmetry) [1, 2, 7].

Gefen et al. [6] briefly explored the critical behavior of magnetic models with continuous $O(n)$ symmetry, $n \geq 2$, on a class of Sierpiński carpets, which are two-dimensional analogues of Menger sponge, and are infinitely ramified. They used a correspondence between electrical properties of a pure resistor network connecting the sites of a lattice and the low-temperature properties of such magnetic models on the same lattice. They established the absence of long range order at finite temperatures in the continuous spin models on fractal structures with $D < 2$, even in the case of an infinite $R$. They speculated that this absence of long range order could be attributed to the fact that the lower critical dimension for spin models with continuous $O(n)$ symmetry on regular lattices is $d = 2$. They remarked that the $O(n)$-model should be examined on fractals with $R = \infty$ and $D > 2$. Recently, we have examined the classical XY-model on a Sierpiński carpet [8], which is a fractal with $R = \infty$ and $D = 1.8928$, and we found no finite-temperature
BKT transition to quasi-long-range order, in agreement with the conjecture of Gefen et al.

Here we examine the classical XY-model on a three-dimensional Menger sponge (MS), Figure 1 which is a fractal structure that has both an infinite $R$ and fractal dimension $D > 2$. The fractal dimension of MS is obtained from the scaling procedure which is used to construct it. One direct iterative process to generate MS begins with the first order ($m = 1$) MS shown in Figure 1 which is obtained by removing from the $2 \times 2 \times 2$ structure the central sites of the six faces and the central site with coordinates (1,1,1). The second order ($m = 2$) MS is then created by translating the first order sponge with 20 translation vectors, which are obtained by multiplying the position vectors of the 20 sites of the first order sponge by a factor of 3. The third order ($m = 3$) MS is obtained by translating the second order sponge with 20 translation vectors which are obtained by increasing the length of the previous set of translation vectors by a factor of 3, etc. Each iteration in this process produces a structure with 20 times more sites than the previous one and with the edge which is three times longer than the edge of the previous structure. From the definition of the fractal dimension $D = \log(\text{number of self-similar pieces})/\log(\text{magnification factor})$ one finds $D = \log(20)/\log(3) = 2.7268$ for the MS.

Similar to a cubic lattice ($R = \infty$), the number of bonds that must be cut to isolate an arbitrarily large cluster of points from the rest of the MS grows as a power of the linear size of the system. Consequently, the MS has an infinite order of ramification.

Since MS is a fractal object, it is scale invariant but not translationally invariant. The deviation from translational symmetry, as well as the degree
of inhomogeneity in the lattice, is measured by the lacunarity $L$. We used a procedure introduced by Gefen et al. [6] to estimate the lacunarity of our fractal, and found it to be $L = 0.19204$ [9].

The Hamiltonian describing our system is given by

\[ H = -J \sum_{\langle i,j \rangle} \cos(\theta_i - \theta_j), \quad (1) \]

where $J > 0$ is the coupling constant, $\langle i,j \rangle$ denotes the nearest neighbors, and $0 \leq \theta_i < 2\pi$ is the angle variable on site $i$. We applied the Wolff cluster algorithm [10] to perform a Monte Carlo study of Eq. (1) on MS of several sizes. In our simulations, we computed the heat capacity, magnetic susceptibility, and helicity modulus for MS of order $m = 1–4$ (the number of sites in a sponge of order $m$ is $20^m$). The dependence of the helicity modulus on the boundary conditions and on system size indicates no finite temperature transition, despite the fact that MS is infinitely ramified and its fractal dimension exceeds the lower critical dimension of the XY-model.

The remainder of the paper is organized as follows. In Section 2 we present our numerical procedure used in calculations. In Section 3 we discuss our results, and summarize our findings in Section 4.

2. Calculation

One procedure for obtaining the MS of order $m$ was described in the Introduction: the sponge of order $m$ is generated by translating the sponge of order $(m-1)$ with 20 translation vectors which are obtained by multiplying the position vectors of the 20 points in the $m = 1$ sponge, shown in Figure 1, by a factor of $3^{m-1}$. The XY-model described by Eq. (1) takes into account only the nearest neighbor interactions, and it is necessary to provide a list of nearest neighbors for each spin on the lattice. By construction of the MS, two sites are nearest neighbors if their distance is equal to 1. It is important to note that since the MS is a fractal object and does not fill space uniformly, the average coordination number varies from one order to another. The sponges of order $m = 1, 2, 3, 4,$ and $5$ have average coordination numbers $2.400, 3.360, 3.744, 3.898,$ and $3.959$, respectively, with standard deviations $0.4899, 0.9113, 1.0181, 1.0532,$ and $1.0659$, respectively. Because of the cubic symmetry of the system, the upper bound on the number of nearest neighbors for any point in the MS is equal to the coordination number of a simple cubic lattice.
Since the fractals lack translational symmetry, we could not employ periodic boundary conditions. Instead we used only the closed boundary condition (CBC) and open (or free) boundary condition (OBC). For the closed boundary condition, each of the eight outer corners of the sponge of order $m$ is coupled to the three closest outer corners, which are located a distance of $3^m-1$ away. For the open boundary condition, the eight outer corners of the sponge are not coupled to each other.

In our simulations we used the Wolff cluster Monte Carlo algorithm [10] because it reduces the problems associated with the critical slowing down observed in the vicinity of a phase transition due to its non-local update scheme. In the Wolff cluster algorithm one starts building a cluster from a randomly chosen site $i$ in the lattice/sponge. At the same time one picks a randomly chosen axis through the origin of the two-dimensional classical planar spin space. All neighboring sites $j$ of $i$ are visited and these sites join the cluster with the probability

$$p_{ij} = 1 - \exp \left( - \frac{J}{k_B T} (s_i^+ s_j^+ + |s_i^+ s_j^+|) \right),$$

(2)

where $s_i^+$ is the component of the spin on site $i$ which is perpendicular to the chosen axis, $k_B$ is the Boltzmann constant, and $T$ is the absolute temperature. Subsequently, one visits the neighbors $k$ of the new sites in the cluster, adding them to the cluster with probability $p_{jk}$ unless they are already in the cluster. This process is repeated until no new sites enter the cluster, at which point one flips the sign of all $s_i^+$ in the cluster, i.e. all spins in the cluster are mirror-reflected in the chosen axis. This completes one Monte Carlo (MC) step in the Wolff algorithm and is analogous to a random change of angle of a single planar spin in the Metropolis MC algorithm [11]. It is clear from Eq. (2) that the average size of clusters of correlated spins increases with decreasing temperature and could approach the system size at sufficiently low temperatures. Hence, the computing time at low temperatures rapidly increases with increasing order of the MS, and we considered only the sponges of order $m \leq 4$.

For sponges of order $m \leq 3$ the simulations typically started at low temperatures and the initial configuration was a “cold” start, such that the system was in its lowest energy state with all the spins aligned. The final configuration at a given temperature was used as the initial configuration for the next higher temperature. For each temperature, we discarded the first 120,000 MC steps (clusters) to allow the system to equilibrate. An additional
7 links, each of 120,000 MC steps, was then generated at each temperature. To get an estimate of the error, we broke each of the 7 links into blocks of 20,000 MC steps. Then the average value was calculated for each of these 42 blocks, and the standard deviation of these 42 averages was used as an estimate of the error.

The largest sponge \((m = 4\) with 160,000 sites) was an exception to this procedure. Seven links of 120,000 MC steps per temperature required more than a month of computing time per temperature for \(k_B T/J < 1.06\). For the largest sponge we started at the highest temperature \(k_B T/J = 1.4\) using a “hot” start, with the spins randomized and the final configuration was used as the initial configuration for the next lower temperature. As in the case of smaller sponges \((m < 4)\), the first 120,000 MC steps (clusters) were discarded and additional 7 links, each of 120,000 MC steps, were generated at each temperature. The lowest temperature at which the data were obtained in this way was \(k_B T/J = 1.06\), and the corresponding CPU time was one month. We obtained an additional set of data at \(k_B T/J = 0.8\) by reducing the size of link from 120,000 MC steps to 30,000 MC steps per link and it took three weeks of CPU time to complete the simulation.

The heat capacity per site was calculated using the fluctuations in internal energy

\[
C = \frac{1}{N} \frac{\langle H^2 \rangle - \langle H \rangle^2}{k_B T^2},
\]

and the linear magnetic susceptibility per site \(\chi\) was calculated from fluctuations in magnetization per site \(m\) as

\[
\chi = \frac{\langle m^2 \rangle - \langle m \rangle^2}{k_B T},
\]

where \(\langle \cdots \rangle\) denotes the MC average.

The helicity modulus for the MS was calculated using the method of Shih, Ebner and Stroud [12] which we used in our previous work [1, 2, 8]. In this scheme, the XY Hamiltonian (Eq. (1)) is thought of as describing a set of Josephson-coupled superconducting grains in zero magnetic field. \(\theta_i\), the direction of spin for each lattice site \(i\), becomes the phase of the superconducting order parameter for that particular site. Applying a uniform vector potential \(A\) causes a shift in the phase difference \(\theta_i - \theta_j\) of the XY Hamiltonian by the amount \(2\pi A \cdot (\mathbf{r}_j - \mathbf{r}_i)/\Phi_0\). In this expression, \(\mathbf{r}_i\) is the position vector of site \(i\), and \(\Phi_0 = hc/2e\) is the flux quantum. The helicity
modulus is then obtained from the second derivative of the Helmholtz free energy per site with respect to uniform $A$, at $A = 0$. The resulting expression for $\gamma$ is

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

(5)

with $H$ the phase-shifted XY Hamiltonian. The vector potential was applied along one of the cube edges of the MS (e.g. x-axis), which amounted to contributions to $\gamma$ only from nearest neighbors whose x-coordinates differ by $\pm 1$ because of the cubic symmetry of the MS.

### 3. Results and Discussion

Our results for the specific heat are shown in Figure 2. In Figure 3 we show the dependence of the maximum in the specific heat $C_{\text{max}}$ obtained with the open boundary condition on the system size. The data were fitted by the formula

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

(6)

and we obtained $C^\infty = 1.36$, $S = -1.35$, and $a = 1.01$, with the $\chi^2$ of the fit equal to $2.03 \times 10^{-7}$. Thus the maximum in the specific heat of the MS saturates in the thermodynamic limit at a value that is not much higher than what we obtained for our largest cluster ($C_{\text{max}} = 1.250 \pm 0.106$ for $N = 160,000$).

The Menger sponge is a structure in three dimensional space but the average coordination number is $\approx 4$ and is in the range characteristic of a two-dimensional system. The specific heat exponent $\alpha$ is not accurately known for the classical XY-model on periodic lattices in $d = 3$. The high-temperature series expansions give $\alpha = -0.02 \pm 0.03$ [13] and $\alpha = 0.02 \pm 0.02$ [14]. The experimental results derived from $C_p$ measurements [15] and from the thermal expansion coefficient measurements [16] near the superfluid transition of $^4$He give $\alpha = -0.02 \pm 0.02$ and $\alpha = -0.026 \pm 0.004$, respectively. Le Guillou and Zinn-Justin [17] have obtained $\alpha = -0.007 \pm 0.006$ using field-theoretical methods. These results seem to favor a small but negative $\alpha$ in which case there is a sharp cusp in the specific heat for an infinite system, and in numerical simulations the specific heat would saturate with increasing system size. On the other hand, the classical XY-model on periodic lattices
in $d = 2$ leads to Berezinskii-Kosterlitz-Thouless (BKT) transition associated with unbinding of topological defects (vortices and antivortices), and the specific heat has an unobservable essential singularity at the transition temperature\cite{[18]}. The Monte Carlo simulations\cite{[19, 20]} give a peak in the specific heat above the BKT transition temperature. The peak is caused by unbinding of vortex clusters\cite{[19]} and its size saturates in the thermodynamic limit\cite{[20]}. We would like to point out that Kohring et al.\cite{[21]} presented Monte Carlo evidence that a continuous phase transition for the classical XY-model on periodic lattices in $d = 3$ is related to unbinding of vortex strings and that the topological defects of this model on the Menger sponge are, in principle, vortex strings in addition to vortices in planes parallel to the faces of the sponge. In our numerical work we did not keep track of topological defects since we did not have an a priori reason to assume that there is a phase transition for the XY-model on the MS.
However, if there is no phase transition for the XY-model on MS, as we eventually conclude based on the data for the helicity modulus, the peak in the specific heat could result from the average energy per site $\langle E \rangle$ changing monotonically from a value slightly higher than $-2J$ (the average coordination number is slightly less than 4) at low temperatures to near zero in disordered paramagnetic phase at high temperatures.

In Figure 4 we show our results for the linear susceptibility of the XY-model on the MS with different number of sites $N$ obtained with both types of boundary conditions. For the classical XY-model on a simple cubic lattice in $d = 3$ the linear susceptibility $\chi$ diverges at transition temperature $k_B T_c/J$ of about 2.2 [26] with the critical exponent $\gamma = 1.316 \pm 0.0025$ [17]. In numerical simulations on finite cubic lattices with periodic boundary conditions one gets a peak in $\chi$ near $k_B T_c/J = 2.2$ whose size and sharpness increase with the number of sites as a result of a diverging correlation length at the onset of long range order [2]. Also, the position of the peak in $\chi$ shows a minute response to the system size, shifting to marginally lower temperatures as the size of the lattice is increased [2]. For the MS we find that the size of the peak in $\chi$ also increases with the system size, the position of the peak shifts to higher temperatures with increasing system size with the open boundary condition, and with the closed boundary condition the position of the peak does not change much with the system size for $N \geq 400$. We note that for the cluster with $N = 8,000$ sites the results for $\chi$ do not
depend much on the boundary condition. For the largest cluster with $N = 160,000$ sites our data at $k_B T / J = 0.8$ and above $k_B T / J = 1.06$ indicate that $\chi$ has a maximum between these two temperatures, not far from $k_B T / J = 0.95$, which is the position of the peak in $\chi$ for the sponge with $N = 8,000$ sites. We note that for the classical XY-model on a square lattice, where the theory \cite{22} predicts diverging susceptibility $\chi$ above the BKT transition temperature and an infinite $\chi$ below the transition temperature, MC simulations give a peak in $\chi$ above the transition temperature whose position is much more sensitive to the system size \cite{1} than in the three-dimensional case. In our work on the XY-model on fractal lattices Sierpiński gasket \cite{1}, Sierpiński pyramid \cite{2}, and Sierpiński carpet \cite{8}, which did not undergo finite temperature phase transition, we found the largest sensitivity in $\chi$ to the system size in terms of both peak height and peak position. Therefore our results for the susceptibility in Figure 4 obtained with the closed boundary condition are not inconsistent with a putative continuous phase transition at
finite temperature.

In our previous Monte Carlo work on the classical XY-model on fractal structures [1, 2, 8] we found the helicity modulus $\gamma(T)$, in particular its dependence on the boundary conditions and on the system size, to be a definitive indicator of presence or absence of a finite temperature phase transition. $\gamma(T)$ provides a measure of the response of a system to a twisting or helical strain at the boundary [23]. A finite resistance to this twist (finite $\gamma$) is expected for a system at zero temperature with all the spins aligned. Conversely, in the high temperature paramagnetic phase with the spins randomized, this rigidity vanishes. In Figure 5 we show the helicity modulus $\gamma(T)$ calculated with the open boundary condition. We find that $\gamma(T)$ vanishes within the error bars for all MS which we considered ($m = 1-4$). The open boundary condition led to vanishing helicity modulus for the XY-model on other fractal structures which we considered in our previous work [1, 2, 8]. That fact, together with the size dependence of the low-temperature $\gamma(T)$ obtained with the closed boundary condition, led us to the conclusion that
there is no finite temperature phase transition in these systems.

The results for the closed boundary condition are presented in Figure 6. As in the cases of the XY-model on Sierpiński gaskets [1], Sierpiński pyramids [2], and Sierpiński carpets [8], the closed boundary conditions lead to finite values of the low-temperature helicity modulus which decrease with increasing system size. One qualitative difference between the results in Figure 6 and those obtained previously is that for Sierpiński gaskets, Sierpiński pyramids, and the Sierpiński carpets the onset of the downturn in $\gamma(T)$ shifted to lower temperatures with increasing system size, but it consistently began around the universal $2/\pi$-line for all system sizes (Nelson and Kosterlitz [24] predicted a universal jump in $\gamma$ at the BKT transition temperature $T_c$ given by $\gamma(T_c)/T_c = 2/\pi$). In the present case, the onset of the downturn in $\gamma$ appears to be unrelated to the $2/\pi$-line, occurring at much higher temperatures, and the onset does not shift substantially to lower temperatures with increasing sponge order. The continuous transition that occurs in the classical XY-model on regular three-dimensional systems is accompa-
nied by power-law decay of $\gamma$ in the vicinity of the transition temperature: $\gamma \propto |T - T_c|^\nu$ with $\nu = 0.662(7)$ \cite{25} for cubic lattices. Also, the low-temperature values of the helicity modulus do not depend on the system size \cite{26}. In MS with the closed boundary condition, the helicity modulus appears to obey power law decay at temperatures below the temperature where it vanishes.

Figure 7 shows a comparison of the thermodynamic quantities for the 8000-site sponge with closed boundary conditions. One can see that similar to cubic lattice, the heat capacity and susceptibility are peaking at roughly the same temperature where the helicity modulus vanishes. Taken on their own these results would suggest that there is a putative continuous phase transition at finite temperature.

However, the low-temperature values of $\gamma$ for MS depend on the system size. In Figure 8 we show the low temperature values of the helicity modulus $\gamma_{\text{max}}$ as a function of the system size and the fit (solid line) according to the
Figure 8: The low temperature values of the helicity modulus calculated with closed boundary condition as a function of the system size.

Formula

\[ \gamma_{\text{max}}(N) = X + \frac{Y}{(\ln N)^f}, \]

with \( X = -0.0045, Y = 2.74, \) and \( f = 1.39, \) and the \( \chi^2 \) of the fit of \( 2.07 \times 10^{-7}. \) These values imply that \( \gamma_{\text{max}} \) vanishes for \( N = 6.4 \times 10^{43}, \) which corresponds to the thermodynamic limit. A fit where \( X \) was set equal to 0 was equally good (dashed line in Figure 8 which overlaps with the solid line). That fit produced \( Y = 2.78 \) and \( f = 1.41, \) with \( \chi^2 \) of the fit of \( 5.72 \times 10^{-7}. \) These results show that the low-temperature value of the helicity modulus obtained with the closed boundary condition goes to zero in the thermodynamic limit \( N \to \infty. \) Hence, we have established numerically that there is no finite temperature phase transition for the classical XY-model on MS.

We should point out that we reproduced all of these results in simulations on the Menger sponges of orders \( m = 1–3 \) using the Metropolis MC algorithm but with slightly larger error bars, except for the heat capacity at high temperatures beyond the maximum in \( C, \) where the Metropolis algorithm produced smaller error bars than the Wolff algorithm.

4. Conclusions

We have performed a Monte Carlo study of the classical XY-model on Menger sponge, which has infinite order of ramification, fractal dimension \( D = 2.7268, \) and lacunarity \( L = 0.19204. \) The open boundary condition
leads to zero helicity modulus at finite temperatures. With the closed boundary condition, the low temperature values of $\gamma$ are finite but decrease with increasing system size. These trends suggest that the closed boundary conditions introduce additional correlations compared to those present in the system with the open boundary condition. By performing the finite-size scaling of the low temperature value $\gamma^{\text{max}}$ of the helicity modulus obtained with the closed boundary condition, we found $\gamma^{\text{max}} = 0$ in the thermodynamic limit $N \to \infty$. Therefore, there is no finite temperature phase transition for the classical XY-model on the Menger sponge, despite the fact that it is infinitely ramified, and has fractal dimension larger than the lower critical dimension of the XY-model. Gefen et al. [6] pointed out that there is no phase transition for spin models with continuous symmetry on a class of Sierpiński carpets with $D < 2$. They suggested that such models should also be investigated on infinitely ramified fractals of fractal dimension $D > 2$ (which is the lower critical dimension of the XY-model). Our work represents such a study and it shows that the value of the fractal dimension $D$ (2.7268 in the present study) cannot be the deciding factor in determining whether or not the phase transition takes place.

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