Thermal behavior of spin clusters and interfaces in the two-dimensional Ising model on a square lattice

Abbas Ali Saberi

School of Physics, Institute for Research in Fundamental Sciences (IPM), PO Box 19395-5531, Tehran, Iran 
E-mail: a_saberi@ipm.ir

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Abstract. An extensive Monte Carlo study of the two-dimensional Ising model is made to investigate the statistical behavior of spin clusters and interfaces as a function of temperature, $T$. We use a tie-breaking rule to define interfaces of spin clusters on a square lattice with strip geometry and show that such definitions are consistent with conformally invariant properties of interfaces at the critical temperature, $T_c$. The effective fractal dimensions of spin clusters and interfaces ($d_c$ and $d_I$, respectively) are obtained as a function of temperature. We find that the effective fractal dimension of the spin clusters varies almost linearly with temperature in three different regimes. It is also found that the effective fractal dimension of the interfaces undergoes a sharp crossover around $T_c$, between the values 1 and 1.75 at low and high temperatures, respectively. We also check the finite-size scaling hypothesis for the percolation probability, and the average mass of the largest spin cluster is in a good agreement with the theoretical predictions.

Keywords: conformal field theory (experiment), stochastic Loewner evolution, classical Monte Carlo simulations, interfaces in random media (experiment)

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The two-dimensional (2D) Ising model, as a solvable prescription model to hand, and its extension to the $q$-state Potts model [1] have been the subject of intensive research interest for decades. Many of their thermodynamical parameters and behaviors can be characterized in terms of some fractal geometrical objects, e.g., spin clusters and domain walls. Most of the studies have been focused on describing the behavior of these models at the critical temperature $T_c$, at which they exhibit a continuous phase transition (for $q \leq 4$), and less attention is paid to investigating the off-critical characterization of such systems at temperatures far from $T_c$. At $T = T_c$, conformal field theory (CFT) plays an important robust role in describing the universal critical properties in two dimensions. Besides CFT, the theory of stochastic Loewner evolution (SLE) invented by Schramm [2] provides a geometrical understanding of criticality which states that the statistics of well-defined domain walls (or curves, e.g., spin cluster boundaries in the 2D Ising model) in the upper half-plane $\mathbb{H}$ is governed by one-dimensional Brownian motion (to review SLE, see [3]). Therefore it is expected that for example in the 2D Ising model, the geometrical exponents such as the fractal dimension of a spin cluster and its boundary as well would be related to the thermodynamical exponents [4]. The study of the fractal structure and the scaling properties of the various geometrical features of the Ising model has been a subject of huge scientific literature (see for example [5]–[9] and references therein). It is also well known that most two-dimensional critical models renormalize onto a Gaussian free field theory (Coulomb gas) [10]. Many exact critical exponents have been computed by using the Coulomb gas technique [11]. These include various geometrical exponents of the two-dimensional Ising model [12], and the general $q$-state Potts model [13,14].

The geometrical objects reflect directly the status of the system in question under changing controller parameters. Temperature can play the role of such a controller parameter in the 2D Ising model.

Investigation of the dependence of geometrical exponents in the 2D Ising model, equivalent to the $q = 2$ states Potts model, is the main subject of the present paper. For consistency with the postulates of SLE at $T = T_c$, we consider the model on a strip of size $L_x \times L_y$, where $L_x$ is taken to be much larger than $L_y = L$, i.e., $L_x = 8L$. We simulate the spin configurations of the 2D Ising model on the square lattice using Wolf’s Monte Carlo algorithm [15], on the basis of single-cluster update. Before going into the further details, let us address an ambiguity that arises when one intends to define an Ising interface on a square lattice, and then introduce a rule which seems to produce well-defined interfaces on the square lattice. The importance of such definitions goes back to its relevance to the SLE interfaces at criticality. As will be discussed later, it is believed that the critical Ising interfaces can be defined by the theory of SLE in the scaling limit [16,17]. Thus we need to have a unique procedure for defining operationally the hulls of the Ising spin clusters without any self-intersection and ambiguity. However we will use our following procedure to define well-defined interfaces in the Ising spin model; one can simply extend it for any two-dimensional model defined on a square lattice, e.g., for interfaces of the general $q$-state Potts model or contour lines of random growth surfaces [18] etc, with appropriate substitutions of up and down spins.

Consider an Ising model on a triangular lattice in the upper half-plane on which each spin lies at the center of a hexagon having six nearest neighbors and the spin boundaries (defining the interface) lie on the edges of the honeycomb lattice (see figure 1). To impose an interface (which separates the spins of opposite magnetization), growing from the origin.
Figure 1. An Ising interface defined on a hexagonal lattice corresponding to a spin configuration on a triangular lattice with a fixed boundary condition at the real line in $\mathbb{H}$, as explained in the text.

Figure 2. An Ising interface defined on a square lattice, the dual of the original square lattice including a spin configuration, with a fixed boundary condition at the real line in $\mathbb{H}$. The interface is generated by applying the turn-right *tie-breaking* rule. The same procedure can be used to define such an interface for down spins ('−') according to the turn-left *tie-breaking* rule.

On the real line to infinity, a fixed boundary condition can be considered in which all spins in the right and left sides of the origin are up ('+') and down ('−'), respectively. The Gibbs distribution induces a measure on these interfaces.

To define an interface, a walker moves on the edges of the hexagonal lattice starting from the origin at the bottom. At each step the walker moves according to the following rule: turn left or right according to the value of the spin in front ('+' or '−', respectively). The resulting interface is a unique interface which never crosses itself and never gets trapped. Such an interface, at $T = T_c$, is believed to be described by SLE in the continuum limit [16, 17].

This procedure for defining the interface should be modified for the spin configuration on a square lattice. This is because there are some choices for the square lattice, at places with four alternating spins. We first introduce a *tie-breaking* rule which the walker regards at each step and then we show that this definition is consistent with the predictions of SLE for such interfaces at $T = T_c$.

Consider a spin configuration on a strip of square lattice in $\mathbb{H}$, with the same boundary conditions as above. A walker moves along the edges of the dual lattice (the lattice shown by the dotted–dashed lines in the figure 2), starting from the origin. According to the
boundary conditions at the first step of the walk, the spins ‘+’ lie to the right of the walker; this direction is chosen to be the preferable direction. After arriving at each site on the dual lattice, there are three possibilities for the walker: it can cross any of the three nearest bonds of the original lattice. At the first step of selection, it chooses the bonds containing two different spins where crossing each of them leaves the spin ‘+’ to the right and spin ‘−’ to the left of the walker. The directions right and left are defined locally according to the orientation of the walker. After the first selection, if there are still two possibilities for crossing, the walker chooses the bond which accords with the turn-right tie-breaking rule: it turns towards the bond which is on its right-hand side with respect to its last direction in the last walk; if there is no selected bond to its right, it prefers to move straight on and if there is also not one there, it turns to its left. The procedure is repeated iteratively until the walker touches the upper boundary. The resulting interface is again an interface which touches itself yet never crosses itself and never gets trapped. The same procedure can be used to define another interface with left-preferable direction as in the turn-left tie-breaking rule.

It is worth mentioning that the procedure introduced here not only yields a unique cluster boundary without any ambiguity on the square lattice, but also one for which it can be checked that any other definition for the interface leads to an incorrect boundary of the cluster. (For example at vertices with more than one possibility, just these introduced options lead to the ‘true’ boundary of the cluster considered, and any other option, for example choosing randomly the directions left or right, may enter the boundary of a spin which does not belong to the cluster. Note that a spin cluster is defined as a set of nearest neighbor connected sites of like sign.)

Let us now show that the resulting interface is compatible with the properties which come from their conformally invariant nature at $T = T_c$.

Wolf’s Monte Carlo algorithm is used to simulate the spin configurations at $T = T_c$, on the strip of the square lattice and of aspect ratio 8, and with boundary conditions as discussed above. For each size $L$, about $4L^2$ Monte Carlo sweeps are used for equilibration. An ensemble of $2 \times 10^4$ independent samples is collected for each sample size $L$, where each of them was taken after $10L$ Monte Carlo steps.

Each spin cluster has been identified as a set of connected sites of the same spin using the Hoshen–Kopelman algorithm. We just take the samples including a vertical spanning cluster in the $y$-direction. Then an ensemble of corresponding spanning interfaces was obtained using the aforementioned turn-right (left) tie-breaking rule.

The fractal dimension of the interfaces at this critical temperature, $d_i(T_c)$, is obtained using the standard finite-size scaling. The length of an interface $l$ scales with the sample size as $l \sim L^{d_i(T_c)}$. The fractal dimension of conformally invariant curves is provided by SLE [3] generally as $d_i = 1 + \kappa/8$, where the diffusivity $\kappa$ classifies different universality classes, and for Ising spin cluster boundaries it is conjectured to be $\kappa = 3$ and thus $d_i(T_c) = \frac{11}{8} = 1.375$. As shown in figure 3, the best fit to our data collected for sizes $30 \leq L \leq 500$ yields the fractal dimension $d_i(T_c) = 1.371 \pm 0.005$.

Another prediction of the theory of SLE for such critical interfaces is the winding angle statistics [2]. We define the winding angle $\theta$ as defined by Wieland and Wilson [19]. For each interface we attribute an arbitrary winding angle to the first edge (that we take zero). Then the winding angle for the next edge is defined as the sum of the winding angle of the present edge and the turning angle to the new edge measured in radians. It
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Figure 3. Log–log plot of the average length of a spanning interface $l$, generated using the tie-breaking rule introduced in the text, versus the width of the strip $L$, at critical points. Main: for the Ising model. Inset: for the hull (the upper graph) and its external perimeter (EP—the lower graph) for critical site percolation. The values of the best fit to the data are represented beside each one, with an error of $\sim 0.005$.

is shown that [19, 20] the variance in the winding grows with the sample size like

$$\langle \theta^2 \rangle = a + \frac{\kappa}{4} \ln L,$$  

(1)

where $\kappa = 8[d_1(T_c) - 1]$, and $a$ is a constant whose value is irrelevant. So the exact value of $\kappa$ for critical interfaces of 2D Ising model should be $\kappa = 3$.

The figure 4 indicates that our result for $\kappa$ is in good agreement with the predicted value. We find that $\kappa = 3.012 \pm 0.005$.

We have also tested other conformally invariant properties of the interfaces such as Schramm’s formula for the left passage probability of the interfaces, which is consistent with the theory (the results are not shown here).

To investigate another concern about the systems with more complicated interfaces, we did such experiments for the critical site percolation [21]. The fractal dimension of the hull and its external perimeter are obtained as $d_1^H = 1.751 \pm 0.002$, and $d_1^{EP} = 1.335 \pm 0.002$, respectively (see figure 3) in good agreement with the duality relation predicted from the conformal invariant property [22]

$$(d_1^H - 1)(d_1^{EP} - 1) = \frac{1}{4}.$$  

(2)

In the rest of the paper, let us consider the statistical geometrical response of the Ising model to the temperature. We show experimentally how the statistics of the spin clusters and their boundaries behave as a function of temperature. We try to measure

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Figure 4. Variance of the winding angle for spanning interfaces generated using the tie-breaking rule introduced in the text. The solid line is set according to equation (1), with $a = -0.29$ and $\kappa = 3$. In the inset, the variance is in semilogarithmic coordinates.

The corresponding fractal dimensions at length scales smaller than the correlation length $\xi$, using the standard finite-size scaling as was done at the critical temperature above.

Features of the spin clusters at three different temperatures are shown in figure 5. These represent what we expect to happen: at zero temperature, because of the boundary conditions used, the ground state of the spin configuration splits the system into two segments, one with spins up and the other with spins down which are separated with a straight interface. Increasing the temperature induces a fractal random feature on spin clusters and interfaces. The interfaces are non-intersecting curves (in $\mathbb{H}$) which can be described, in the continuum limit, by means of a dynamical process called Loewner evolution [23] with a suitable continuous driving function $\zeta_t$ given as

$$\frac{\partial g_t(z)}{\partial t} = 2 \frac{g_t(z) - \zeta_t}{g_t(z) - \zeta_t},$$

where, if we consider the hull $K_t$, the union of the curve and the set of points which cannot be reached from infinity without intersecting the curve, then $g_t(z)$ is an analytic function which maps $\mathbb{H} \setminus K_t$ into $\mathbb{H}$ itself.

At zero temperature the driving function $\zeta_t$ is a specific constant; at $T = T_c$ it should be proportional to a standard Brownian motion $B_t$ as $\zeta_t = \sqrt{\kappa}B_t$ with $\kappa = 3$, and it may be a complicated random function at other different temperatures.

At the limit of high temperature, each spin gets the directions up or down with probability $p = 1/2$ and so it is conjectured to correspond to the critical site percolation on a triangular lattice (on which the percolation threshold is exactly $p_c = 1/2$), and the driving function is expected to converge to a Brownian motion with the diffusivity of $\kappa = 6$. For the case of a square lattice, since the percolation threshold in two dimensions
Figure 5. Spin clusters of the 2D Ising model on a strip of a square lattice with size of $L = 120$, and aspect ratio 6, at different temperatures from top to bottom: $T - T_c = -0.2, 0$ and, $0.2$. The boundary conditions (bc) used for simulation are fixed for the lower boundary, antiperiodic at the sides and free for the upper part. The spin down clusters are shown white. The bc imposes an interface at the boundary of the spanning cluster (dark colored) starting from the origin (using the turn-left *tie-breaking* rule in these figures) and ending at the upper boundary. As temperature increases the interface gets more space filling.

is at $p_c \sim 0.59$, at the limit of high temperature, where $p = \frac{1}{2} < p_c$, the system will be below the threshold and the crossover to the critical site percolation will not be seen any longer.

Before looking at the temperature dependence of the fractal dimension of the spin clusters, let us discuss more their scaling properties from the point of view of theoretical expectations.

The Ising model is expected to be scale invariant (on scales much larger than lattice spacing $a$) only at renormalization group fixed points, i.e., $T = T_c$ and $\infty$ (on the triangular lattice). At those points one expects well-defined power-law behavior for clusters and their hulls on all scales $L \gg a$. For $T$ just above $T_c$, where the correlation length $\xi$ is finite and $\xi \gg a$, one expects to see behavior characteristic of the critical point $T_c$ on scales $a \ll L \ll \xi$, and of the fixed point for high temperature on scales $L \gg \xi$.

Thus, according to the theory, there should be no such thing as ‘the fractal dimension at temperature $T$’, except for $T = T_c$ and $\infty$; instead one should see a crossover between two different values. If one chooses a sufficiently narrow range of length scales one will see an effective fractal dimension, which will have the appearance of depending on temperature. However, for the Ising model on a square lattice, since the crossover to the critical percolation at high temperatures no longer exists, the behavior of the effective fractal dimensions is governed by just the behavior at $T = T_c$ for length scales $a \ll L \ll \xi$. In order to determine the behavior of such effective fractal dimensions as a function of temperature, we measure them in a fairly narrow range of sizes $L$, which seem to be much
smaller than the correlation length and within the range in which the scaling properties hold.

Figure 6 shows the procedure that we perform to measure the effective fractal dimension of the spin clusters and interfaces at different temperatures. The finite-size scaling substantially reduces the statistical errors in estimating the fractal dimensions. The average is taken over $10^4$ independent samples of aspect ratio 4, at each temperature below $T_c$ for each sample size (only the spanning cluster in each configuration and the corresponding interface were considered). Since the probability of having a spanning cluster diminishes when temperature increases (as will be discussed later), the average is taken over $2 \times 10^4$ independent samples for $T > T_c$, and the samples were gathered on a strip of aspect ratio 8.

The exact values for the fractal dimensions of spin clusters and interfaces are known just for at the critical temperature $T_c$, as $d_c(T_c) = \frac{187}{96} = 1.9479 \ldots$ and $d_I(T_c) = \frac{11}{8} = 1.375$, respectively. Our measurements of fractal dimensions at $T_c$ which give $d_c(T_c) = 1.9469 \pm 0.001$ and $d_I(T_c) = 1.371 \pm 0.005$ are in a good agreement with the exact results. These values were obtained for $30 \leq L \leq 500$. The same measurements for $T \neq T_c$ were done for 10 different sizes within $50 \leq L \leq 500$ (the examples are shown in figure 6).
Figure 7. Effective fractal dimension of spin clusters as a function of temperature. It changes almost linearly in three different regimes: low temperature with the dimension of 2, rapid decreasing around $T_c$ and a crossover to a different linear behavior far from $T_c$. The slope of the dashed lines differs by one order of magnitude. Each point is obtained using finite-size scaling for 10 different sizes in the range of $50 \leq L \leq 500$. The error is less than the symbol size.

Figure 6 shows the scaling properties and the fractal behavior of the spin clusters and interfaces at $T \neq T_c$, within the selected range of size.

To quantify the geometrical changes of the spin clusters at different temperatures, we measure the effective fractal dimensions of the spin clusters and their perimeters. At each temperature, we use the scaling relation between the average mass of the spanning spin cluster $M$, and the width of the strip $L$, to measure the fractal dimension of the spin clusters—i.e., $M \sim L^{d_c}$.

The corresponding fractal dimension of spin clusters as a function of temperature is shown in figure 7. This suggests three different regimes. One is for low temperatures in which the dimension of the spin clusters is 2. The second regime is in the vicinity of the critical temperature: a linear dependence of the fractal dimension on temperature with a sharp decrease which is governed by criticality. A crossover happens at temperature above the critical region which changes the slope of the linear decrease by about one order of magnitude at high temperatures.

Such a crossover can also be seen in the behavior of the effective fractal dimension of the interfaces as a function of temperature. As shown in figure 8, at low temperatures the effective fractal dimension of the interfaces is close to 1 and it increases with temperature. In the vicinity of the critical temperature it increases again sharply and then crosses over to a value very close to 1.75, which is the fractal dimension of the hull of critical
percolation. The whole behavior looks like a hyperbolic tangent function. The other theoretical predictions for the geometrical features that are considered in this paper, and that we are interested in checking, concern the percolation observables. The finite-size scaling hypothesis states that the percolation probability \( P_s \), i.e., the probability of having a spanning cluster at temperature \( T \), reaching from one boundary to the opposite one, behaves like \[ P_s = P_s(L/\xi), \] (4)

where the correlation length behaves like \( \xi \sim (T - T_c)^{-\nu} \), with \( \nu = 15/8 \) for the Ising spin geometric clusters.

In order to investigate this hypothesis, we have done simulations of the Ising model on square lattices of different sizes \( L^2 \) with free boundary conditions, and the measurements are taken by averaging over \( 2 \times 10^4 \) independent samples at each temperature. As shown in figure 9, curves \( P_s \) measured on lattices of different size all cross at the critical point (in the figure this observable is shown as a function of the inverse temperature \( \beta \)). As can be seen from the figure, applying the scaling theory equation (4), the data collapse onto a single function, in a good agreement with the theoretical predictions.

The other observable that we consider is the scaling behavior of the average mass of the largest spin cluster, \( M \). According to theory, this should have the scaling form

\[ M = L^{d_c(T_c)} F(L/\xi), \] (5)

where the scaling function \( F(x) \) goes to a constant as \( x \to 0 \) (at \( T = T_c \)).

The suitably rescaled mass of the largest spin cluster as a function of the reduced inverse temperature is plotted in figure 10, implying data collapse onto a universal curve.
Figure 9. Finite-size scaling plots of the data for the percolation probability, measured on square lattices of different sizes $L^2$. Inset: the percolation probability as a function of the inverse temperature $\beta$.

Figure 10. Data collapse for the average mass of the largest spin cluster $M$, measured on square lattices of different sizes $L^2$. Inset: the strength of the largest spin cluster as a function of the inverse temperature $\beta$. 
In conclusion, we have studied the geometrical changes of the spin clusters and interfaces of the two-dimensional Ising model on a square lattice in the absence of an external magnetic field, as a function of temperature. We introduced a well-defined tie-breaking rule to generate non-intersecting interfaces on a square lattice, which are shown to be consistent with the predictions of conformal invariance at the critical point. The results are also checked for critical site percolation and found to be in good agreement with the analytical predictions.

We also investigated the effect of the temperature on the statistical properties of geometrical objects by measuring the effective fractal dimensions of the spin clusters and interfaces as a function of temperature. We showed that a crossover happens which distinguishes between the behavior of these geometrical objects near the critical temperature and that of at high temperatures.

We also applied the finite-size scaling hypothesis for both the percolation probability and the average mass of the largest spin cluster, and we found a data collapse onto a universal curve, in good agreement with the theoretical predictions.

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