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LETTER TO THE EDITOR

Droplets in the two-dimensional critical Ising model and conformal invariance

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Abstract. The equilibrium form of droplets at a wall and around a fixed interior spin in the two-dimensional critical Ising model is derived using conformal invariance methods. The results are in good agreement with Monte Carlo simulations.

In this letter the two-dimensional Ising model with the boundary conditions shown in figures 1(a) and 1(b) is considered. The Ising model of figure 1(a) is semi-infinite and has fixed boundary spins, all of which are positive except for L adjacent negative spins. Figure 1(b) depicts a finite $N \times N$ Ising model with positive boundary spins and one fixed negative spin at the centre.

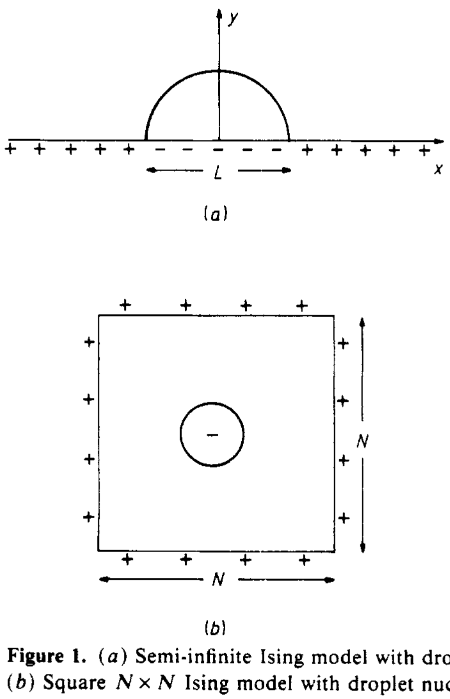

Figure 1. (a) Semi-infinite Ising model with droplet nucleated by L adjacent down spins. (b) Square $N \times N$ Ising model with droplet nucleated by a fixed spin at the centre.

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The fixed negative spins in figure 1 nucleate extended droplets of negative local magnetisation. For $L \gg 1$ and $T < T_c$ the shape of the droplet at a wall corresponding to figure 1(a) is presumably elliptical, as follows from SOS interface models [1, 2] and random walk [3] arguments. For $L \gg 1$ the droplet radius extends a distance of order $L^{1/2}$ lattice constants from the boundary. These results are consistent with Abraham's exact expression [4] for the magnetisation profile of the Ising model along the symmetry axis $x = 0$ of the droplet and with Monte Carlo simulations of the Ising and three-state Potts models with the boundary geometry of figure 1(a) by Selke [5].

In [5] simulations of an interior droplet for the boundary geometry of figure 1(b) are also reported. At the bulk critical temperature T_c the droplet becomes circular in the large-N limit, and its radius is given by

$$R = cN^{1/2} \qquad N \gg 1. \tag{1}$$

The exponent $\frac{1}{2}$ in equation (1) follows [5] from a model-independent finite-size scaling argument.

In this letter the exact local magnetisation of the two-dimensional Ising model with the two boundary conditions shown in figure 1 is derived using conformal invariance [6] methods. The results hold at the bulk critical temperature T_c in the continuum limit L, $N \gg 1$. At T_c the droplet at a wall has a semicircular shape with radius $L/2$, as compared with an elliptical shape with semi-axis of order $L^{1/2}$ for $T < T_c$. Conformal invariance confirms equation (1) and implies $c = 0.181\,671$ for the proportionality constant. These predictions are compared with Monte Carlo simulations, and good agreement is found.

First we derive the magnetisation $m_L(x, y)$ for the boundary conditions of figure 1(a). The mixed boundary conditions along the x axis may be replaced by a uniform spin-up boundary condition if an antiferromagnetic seam of length L is inserted along the x axis. Introducing the antiferromagnetic seam with disorder operators [7], we express the magnetisation in the form

$$m_L(x, y) = \lim_{y_0 \to 0} \frac{\langle \sigma(x, y)\mu(L/2, y_0)\mu(-L/2, y_0)\rangle}{\langle \mu(L/2, y_0)\mu(-L/2, y_0)\rangle}. \tag{2}$$

Here $\sigma(x, y)$ and $\mu(x, y)$ denote Ising spin and disorder variables, respectively. The correlation functions in equation (2) are evaluated with uniform spin-up boundary conditions along the x axis.

By duality [8] the two-point correlation function in equation (2) is the same as the spin–spin correlation function in the half space with free-spin boundary conditions. This function, calculated by Cardy [9], is given in equation (10) below. The three-point function in equation (2) was derived by Burkhardt and Guim [10]. Inserting the results in equation (2), we obtain

$$m_L(x, y) = A^{1/2}(y/2)^{-1/8}\{1 - y^2L^2[(x - L/2)^2 + y^2]^{-1}[(x + L/2)^2 + y^2]^{-1}\}^{1/2} \tag{3}$$

for the local magnetisation corresponding to the droplet at a wall. The numerical value of the constant A is given in equation (12). From equation (3) one sees that the magnetisation vanishes on the curve

$$x^2 + y^2 = (L/2)^2. \tag{4}$$

Thus, as mentioned above, the droplet is semicircular, with radius $L/2$.

Next we consider the magnetisation profile $m_N(\boldsymbol{r})$ for the boundary geometry of figure 1(*b*), defined by the thermal average

$$m_N(\boldsymbol{r}) = \lim_{h\to\infty} \frac{\mathrm{Tr}\{\sigma(\boldsymbol{r}) \exp[-\beta H - h\sigma(\boldsymbol{o})]\}}{\mathrm{Tr}\exp[-\beta H - h\sigma(\boldsymbol{o})]}. \tag{5}$$

Here the central spin $\sigma(\boldsymbol{o})$ has been explicitly fixed by application of a local field h. For Ising spins that take the values $\sigma = \pm 1$, $\exp(-h\sigma) = (1-\sigma \tanh h)\cosh h$. Substituting this identity into equation (5) and taking the limit $h \to \infty$, we obtain

$$m_N(\boldsymbol{r}) = \frac{\langle\sigma(\boldsymbol{r})\rangle - \langle\sigma(\boldsymbol{r})\sigma(\boldsymbol{o})\rangle}{1-\langle\sigma(\boldsymbol{o})\rangle}. \tag{6}$$

Equation (6) expresses the droplet magnetisation $m_N(\boldsymbol{r})$ in terms of one- and two-point functions for the square geometry with fixed boundary spins but with no restrictions on the central spin.

To see the origin of the exponent $\frac{1}{2}$ in equation (1), note that

$$\langle\sigma(\boldsymbol{r})\rangle \simeq \langle\sigma(\boldsymbol{o})\rangle \simeq BN^{-\beta/\nu} \tag{7}$$

for $1 \ll r \ll N$, as follows from finite-size scaling [11]. In this asymptotic regime

$$\langle\sigma(\boldsymbol{r})\sigma(\boldsymbol{o})\rangle \simeq Ar^{-2\beta/\nu} \tag{8}$$

reduces to the bulk pair correlation function. Substituting equations (7) and (8) into (6), one sees that $m_N(\boldsymbol{r})$ vanishes at a droplet radius given by equation (1), with $c = (A/B)^{\nu/2\beta}$. The square-root law (1), first derived in [5], holds for an interior droplet in an arbitrary critical system with characteristic size $N \gg 1$.

An explicit formula for $m_N(\boldsymbol{r})$, analogous to equation (3), may be obtained by conformal mapping of known correlation functions for the half-space according to [6]

$$\langle\sigma(w_1)\sigma(w_2)\ldots\rangle = |w'(z_1)w'(z_2)\ldots|^{-\beta/\nu}\langle\sigma(z_1)\sigma(z_2)\ldots\rangle. \tag{9}$$

Here $z = x + \mathrm{i}y$ and $w = u + \mathrm{i}v$ are complex position coordinates, and w is an analytic function of z.

For the Ising model defined on the half-space $y > 0$, Cardy [6, 9] has obtained

$$\langle\sigma(z_1)\sigma(z_2)\rangle = A(4y_1y_2)^{-1/8}(\tau^{1/4} \pm \tau^{-1/4})^{1/2} \tag{10a}$$

$$\tau = [(x_1-x_2)^2 + (y_1+y_2)^2]/[(x_1-x_2)^2 + (y_1-y_2)^2] \tag{10b}$$

for the two-point function. The upper and lower signs correspond to fixed and free boundary spins, respectively. The correlation function is normalised to reduce to the bulk result (8) for $y_1y_2 \gg (x_1-x_2)^2 + (y_1-y_2)^2$. For $y_1y_2 \ll (x_1-x_2)^2 + (y_1-y_2)^2$, $\langle\sigma(z_1)\sigma(z_2)\rangle$ factors as $\langle\sigma(z_1)\rangle\langle\sigma(z_2)\rangle$, with

$$\langle\sigma(z)\rangle = A^{1/2}(y/2)^{-1/8} \tag{11}$$

in the case of fixed boundary spins. For the Ising model on a square lattice with unit lattice constant, the amplitude A in equations (8), (10), and (11) has the numerical value [12]

$$A = 2^{1/8}(0.645\,002\,448). \tag{12}$$

The analytic function

$$w(z) = K\int_0^z [(1-t^2)(1-k^2t^2)]^{-1/2}\,\mathrm{d}t \tag{13}$$

with $0<k<1$ and real, maps [13] the half plane $\Im z>0$ onto the rectangle $-w(1)<u<w(1)$, $0<v<w(k^{-1})$. An explicit expression for $m_N(\boldsymbol{r})$ in terms of incomplete elliptic integrals may be obtained by choosing K and k so that $2w(1)=w(k^{-1})=N$ and then substituting equations (9)-(13) into (6).

We now consider the calculation of the proportionality constant c in equation (1). As noted below equation (8), $c=(A/B)^{\nu/2\beta}$, where A and B are defined by equations (7) and (8). From (7), (9) and (11) with $\beta/\nu=\frac{1}{8}$, it follows that

$$\langle\sigma(\boldsymbol{o})\rangle = A^{1/2}|y_0 w'(z_0)/2|^{-1/8} = BN^{-1/8}. \tag{14}$$

Thus the droplet radius is given by equation (1) with

$$c = A^2|y_0 w'(z_0)/2N|^{1/2}. \tag{15}$$

Equations (1) and (15) are not limited to the square geometry, but hold for a droplet in any domain of characteristic size N onto which the upper half plane can be conformally mapped. The point z_0 is the particular point in the half plane that maps onto the centre of the droplet.

For $k^2=17-12\sqrt{2}$, $\frac{1}{2}$ and 1, equation (13) maps the upper half plane onto $N\times N$, $N\times 2N$ and $N\times\infty$ rectangles, respectively [13, 14]. For general k the point $z_0=\mathrm{i}y_0=\mathrm{i}k^{-1/2}$ maps onto the centre of the rectangle. Combining equations (12), (13) and (15), we obtain $c=0.181\,671$, $0.196\,440$ and $0.197\,374$ for the $N\times N$, $N\times 2N$ and $N\times\infty$ rectangles, respectively. (The value of c for the $N\times\infty$ rectangle or strip also follows directly from the mapping $w=(N/\pi)\ln z$.) One sees that c is fairly insensitive to the aspect ratio of the rectangle.

The radius R of a droplet at the centre of the Ising model on a square lattice with unit lattice constant and a circular boundary of radius N is also given by equation (1), with $c=0.247\,372$. This follows from the mapping $w=N(z-\mathrm{i})/(z+\mathrm{i})$ of the half plane $\Im z>0$ onto the disc $|w|<N$.

We now compare the theoretical predictions with Monte Carlo results. In our new simulations of the droplet at a wall, $N\times N$ systems were considered, as shown in figure 2. At criticality very long runs were necessary to obtain reliable equilibrium data. The first 40 000 to 150 000 Monte Carlo steps per spin were discarded. In calculating averages two or more runs, each of 150 000 to 300 000 Monte Carlo steps per spin, were performed, with the shorter runs for smaller systems. Further procedural details are the same as in [5].

The Monte Carlo results for the semi-axis y_m of the Ising droplet at a wall are indicated by the filled circles in figure 2. For the larger base lengths $L=11$ and 15, the data extrapolate in the large-N limit to values in excellent agreement with the prediction $y_m=L/2$ (see equation (4)) of conformal invariance. As mentioned above, this prediction holds in the continuum limit $L\gg 1$. For the smaller base lengths $L=5$ and 7, the extrapolated y_m appears to be slightly less than $L/2$.

Next we compare the square-root law (1) with $c=0.181\,671$ for the Ising droplet around a fixed central spin in an $N\times N$ system with the Monte Carlo data in figure 9 of [5]. The straight-line fit to the Ising data in figure 9 corresponds to $c\simeq 0.20$, which is a little larger than the theoretical prediction. The slight discrepancy may be due to finite-size corrections. (Equations (6) and (9)-(12) imply that the leading correction as $N\to\infty$ to the right-hand side of equation (1) is a geometry-independent additive constant 0.122 386.) For $N=200$, the largest N considered in the simulations, the droplet radius R is only about three lattice constants. Thus most of the data do not

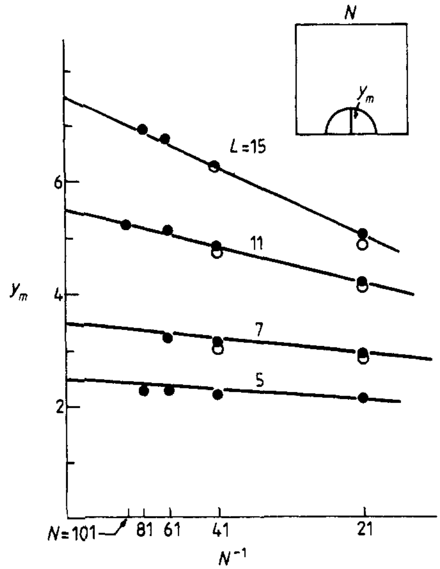

Figure 2. Monte Carlo results for the semi-axis y_m of a droplet of base length L at a wall in $N \times N$ Ising (filled circles) and three-state Potts (open circles) models. The straight lines intersect the y_m axis at the theoretical prediction $y_m = L/2$, $L \gg 1$ for the Ising model and pass through the Ising data points at $N = 21$. The uncertainty in the data points is comparable to their diameter.

satisfy the condition $R \gg 1$ (continuum limit) assumed in the conformal invariance approach.

In the critical three-state Potts model one also expects droplet sizes proportional to L and $N^{1/2}$ for the boundary geometries of figures 1(a) and 1(b), respectively. This is confirmed by the Monte Carlo data shown in figure 2 (open circles) of this paper and in figure 9 of [5]. According to the Monte Carlo results the proportionality constants for the three-state Potts and Ising models are quantitatively very close, i.e. $y_m \simeq L/2$ and $c = 0.19 \pm 0.01$ in both models. Extending our analytical approach to the three-state Potts model is unfortunately rather difficult. The two- and three-spin correlation functions in the half-space [15] needed to predict the droplet form have not yet been calculated. In the conformal theory of the three-state Potts model these correlation functions are determined by sixth-order differential equations, as compared with second-order for the Ising model [6].

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