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Geometry of Equilibrium Configurations in the Ising Model

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We derive microscopically precise identities for the geometry of small clusters in the equilibrium states of the two-dimensional Ising model with emphasis on near-critical phenomena.

KEY WORDS: Two-dimensional Ising model; equilibrium; cluster geometry.

In this note we express the densities $d_k^{\pm}$ of $(\pm)$ lattice sites with k $(-)$ neighbors as linear combinations of the 1 to 5 point correlations (Section 1), compute their equilibrium expectations $\langle d_k^{\pm} \rangle$ at temperatures β^{-1} (Section 2) and infer from them the equilibrium densities of small clusters and various other cluster properties (Section 3). Of special interest are the phenomena which occur at the critical point $\beta_c^{-1} \sim 0.44$ at which the functions $\langle d_k^{\pm} \rangle(\beta)$ change abruptly and bifurcate (Fig. 1).

1. DENSITY OF LOCAL CONFIGURATIONS

For any spin configuration ω on the sites of a two-dimensional square lattice Λ consider the *local observables*

$$d_k^{\pm}(\omega, x) = \begin{cases} 1 & \text{if} \quad \omega(x) = \pm 1 \quad \text{and } x \text{ has } k \text{ nearest } (-) \text{ neighbors} \\ 0 & \text{otherwise} \end{cases}$$

For $k = 2$ there are two distinct possibilities

$$d_2^{\pm}(\omega, x) = {}^a d_2^{\pm}(\omega, x) + {}^0 d_2^{\pm}(\omega, x)$$

with ${}^a d_2$ and ${}^0 d_2$ corresponding to the cases where the two $(-)$ neighbors are adjacent and opposite, respectively.

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By $s_{\alpha\beta\gamma\ldots}(\omega, x)$ we denote the rotation-averaged products of ω at the locations α, $\beta, \gamma \ldots$ indicated by the picture

	2	
3	0	1
	4	

An elementary derivation shows that the quantities $d_k^{\pm}(\omega, x)$ are the following linear combinations of the 1 to 5 point *correlations* $s \ldots (\omega, x)$:

	1	s_1	s_{01}	s_{12}	s_{13}	s_{012}	s_{013}	s_{123}	s_{0123}	s_{1234}	s_{01234}
$32\, d_0^{\pm}$	1	4 ± 1	± 4	4	2	± 4	± 2	4	± 4	1	± 1
$32\, d_1^{\pm}$	4	8 ± 4	± 8	0	0	0	0	-8	∓ 8	-4	∓ 4
$32\, {}^a d_2^{\pm}$	4	± 4	0	0	-8	0	∓ 8	0	0	4	± 4
$32\, {}^0 d_2^{\pm}$	2	± 2	0	-8	4	∓ 8	± 4	0	0	2	± 2
$32\, d_3^{\pm}$	4	-8 ± 4	∓ 8	0	0	0	0	8	± 8	-4	∓ 4
$32\, d_4^{\pm}$	1	-4 ± 1	∓ 4	4	2	± 4	± 2	-4	∓ 4	1	± 1

(1.1)

The 12 identities (1.1) hold at each site and for any ω and therefore for averages over all sites or with respect to any distributions of ω's. They hold in particular for the densities

$$d_k^{\pm}(\omega) = \frac{1}{|\Lambda|} \sum_{x \in \Lambda} d_k^{\pm}(\omega, x), \qquad s \ldots (\omega) = \frac{1}{|\Lambda|} \sum_{x \in \Lambda} s \ldots (\omega, x)$$

Let

$$m(\omega) = s_1(\omega), \qquad l(\omega) = 1 - s_{01}(\omega)$$

denote the average magnetization and boundary length (number of unlike neighbor pairs) per site, and

$$d_k(\omega) = d_k^{+}(\omega) + d_k^{-}(\omega)$$

the density of sites with k $(-)$ neighbors. Then

$$\begin{gathered}
\sum_{k=0}^{4} d_k(\omega) = 1 \\
\sum_k k d_k(\omega) = 2(1 - m(\omega)) \\
\sum_k (d_k^{+}(\omega) - d_k^{-}(\omega)) = m(\omega) \\
\sum_k k d_k^{+}(\omega) = l(\omega)
\end{gathered} \tag{1.2}$$

These identities, which hold for all possible configurations, have an obvious geometrical meaning and can be verified directly.

2. EQUILIBRIUM EXPECTATIONS

The expectations $\langle s_0\rangle, \langle s_{01}\rangle, \langle s_{12}\rangle, \langle s_{13}\rangle$ of the 1- and 2-point correlations in the Gibbs state

$$\rho_0(\omega) = Z^{-1}e^{-\beta H(\omega)}, \qquad H(\omega) = -J \sum_{|x-y|=1} \omega(x)\omega(y)$$

are well-known.[1] From these the higher-order correlations are obtained by the *Fisher identities*[2,3]: Let

$$\varphi = \tanh(2\beta J), \qquad \psi = \tanh(\beta J)$$

then

$$\langle s_{012}\rangle = \frac{\varphi(1-2\psi)}{\varphi - 2\psi}\langle s_1\rangle = \langle s_{013}\rangle$$

$$\langle s_{123}\rangle = \frac{2-\varphi-2\psi}{\varphi-2\psi}\langle s_1\rangle$$

$$\langle s_{1234}\rangle = \frac{2}{\varphi-2\psi}\left[\varphi - \psi + 2\langle s_{01}\rangle - \varphi(2\langle s_{12}\rangle + \langle s_{13}\rangle)\right]$$

Denoting

$$\langle s_1\rangle = m, \qquad \langle s_{01}\rangle = s_{01}, \qquad 2\langle s_{12}\rangle + \langle s_{13}\rangle = a$$

we obtain from (1.1) the following *equilibrium expectations*:

$$\begin{aligned}
d_0 &= \frac{1}{8(2\psi-\varphi)}\left[2\psi(1+a) - 4s_{01} + 4(2\psi-1)m\right] \\
d_1 &= \frac{4}{8(2\psi-\varphi)}\left[-\varphi(1+a) + 4s_{01} + 2(1-\varphi)m\right] \\
d_2 &= \frac{6}{8(2\psi-\varphi)}\left[2\psi(1+a) - 4s_{01}\right] - a \\
d_3 &= \frac{4}{8(2\psi-\varphi)}\left[-\varphi(1+a) + 4s_{01} - 2(1-\varphi)m\right] \\
d_4 &= \frac{1}{8(2\psi-\varphi)}\left[2\psi(1+a) - 4s_{01} - 4(2\psi-1)m\right]
\end{aligned} \tag{2.1}$$

Also, at equilibrium, one can show that

$$d_k^{\pm} = \frac{1}{2}\left[1 \pm \tanh(2\beta J(2-k))\right]d_k \tag{2.2}$$

So all ten geometric observables can be calculated from the three functions m, s_{01}, a.

Using the integrals for m, s_{01}, a from Ref. 1, p. 199, we have computed the d_k's as functions of β (Fig. 1, Table I).

In the limit $\beta \to 0$ (2.1) yields

$$d_0 = d_4 = 1/16, \qquad d_1 = d_3 = 4/16, \qquad d_2 = 6/16 \tag{2.3}$$

and a counting argument shows that they correspond to the expected values in the random state.

At supercritical temperatures $\beta < \beta_c$ we know that the expected magnetization vanishes. From (2.1) it follows, for $m = 0$, that

$$d_k = d_{4-k} \tag{2.4}$$

Figure 1 moreover shows that $d_0 = d_4$ increase, and $d_1 = d_3, d_2$ decrease monotonically, for increasing β.

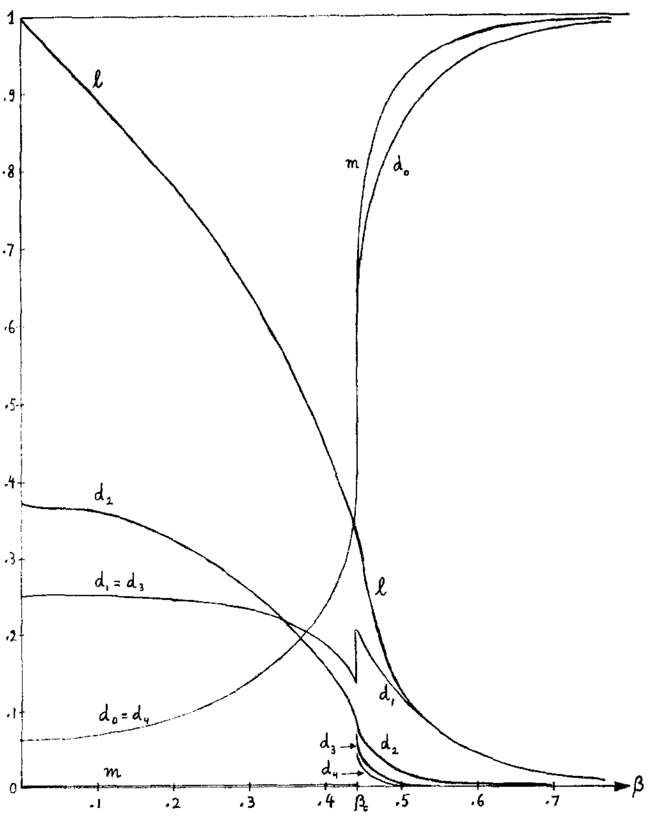

Fig. 1. Diagram of the functions $d_k(\beta)$.

Table I. Equilibrium Expectations of m, l, and d_k (Ferromagnet)

β	m	l	d_0	d_1	d_2	d_3	d_4
0.0	0.0	1.0	0.0625	0.2500	0.3750	0.2500	0.0625
0.05	0.0	0.9498	0.0630	0.2542	0.3656	0.2542	0.0630
0.1	0.0	0.8983	0.0689	0.2501	0.3621	0.2501	0.0689
0.15	0.0	0.8442	0.0775	0.2491	0.3469	0.2491	0.0775
0.2	0.0	0.7859	0.0905	0.2470	0.3248	0.2470	0.0905
0.25	0.0	0.7214	0.1094	0.2424	0.2964	0.2424	0.1094
0.3	0.0	0.6478	0.1361	0.2334	0.2610	0.2334	0.1361
0.35	0.0	0.5601	0.1744	0.2168	0.2175	0.2168	0.1744
0.4	0.0	0.4470	0.2329	0.1864	0.1615	0.1864	0.2329
0.45	0.7493	0.2935	0.6905	0.1948	0.0605	0.0307	0.0232
0.5	0.9113	0.1272	0.8541	0.1218	0.0182	0.0045	0.0014
0.55	0.9539	0.0744	0.9171	0.0751	0.0065	0.0011	0.0002
0.6	0.9736	0.0455	0.9504	0.0468	0.0025	0.0003	0.0
0.65	0.9841	0.0285	0.9694	0.0295	0.0010	0.0001	0.0
0.7	0.9902	0.0181	0.9808	0.0188	0.0004	0.0	0.0
0.75	0.9938	0.0117	0.9878	0.0121	0.0002	0.0	0.0
0.8	0.9960	0.0076	0.9921	0.0078	0.0001	0.0	0.0

Table II. Equilibrium Expectations of $d_k^{\pm}$ (Ferromagnet)

β	$d_0^{\pm}$	$d_1^{\pm}$	$d_2^{\pm}$	$d_3^{\pm}$	$d_4^{\pm}$
0.1	0.0475	0.1497	0.1811	0.1004	0.0213
	0.0213	0.1004	0.1811	0.1497	0.0475
0.2	0.0753	0.1704	0.1624	0.0766	0.0152
	0.0152	0.0766	0.1624	0.1704	0.0753
0.3	0.1248	0.1794	0.1305	0.0540	0.0113
	0.0113	0.0540	0.1305	0.1794	0.1248
0.4	0.2238	0.1552	0.0808	0.0313	0.0091
	0.0091	0.0313	0.0808	0.1552	0.2238
0.5	0.8387	0.1073	0.0091	0.0005	0.0
	0.0154	0.0145	0.0091	0.0040	0.0014
0.6	0.9426	0.0429	0.0012	0.0	0.0
	0.0078	0.0039	0.0012	0.0003	0.0
0.7	0.9772	0.0177	0.0002	0.0	0.0
	0.0036	0.0011	0.0002	0.0	0.0
0.8	0.9905	0.0075	0.0	0.0	0.0
	0.0016	0.0003	0.0	0.0	0.0

At the critical point $\beta = \beta_c$ the curves $d_0 = d_4$ and $d_1 = d_3$ bifurcate, reflecting the bifurcation of m. (Figure 1 corresponds to the positive branch of magnetization; for the negative branch d_k should be replaced by d_{4-k}.)

At subcritical temperatures $\beta > \beta_c$, d_0 continues to increase, whereas d_2, d_3, d_4 decrease monotonically. d_1 first increases like d_0 and then also decreases. For positive m, the limits

$$d_0 = 1, \qquad d_1 = d_2 = d_3 = d_4 = 0$$

are reached in the limit $\beta \to \infty$.

From Eq. (2.2) we have also computed the equilibrium expectations of $d_k^{\pm}(\beta)$ (Table II). At supercritical temperatures they exhibit the symmetries

$$d_k^{\pm}(\beta) = d_{4-k}^{\mp}(\beta), \qquad \beta < \beta_c \tag{2.5}$$

3. CLUSTER GEOMETRY

In the *ferromagnetic case* ($J > 0$) the values of d_k at equilibrium are characteristic for the degree of ferromagnetic clustering. Since these values vary rapidly at the critical temperature, one expects drastic critical effects on the cluster properties.

Owing to translation and rotation invariance of the Hamiltonian, we expect the clusters in the asymptotic configurations to be randomly distributed over space. The question then arises how much information about cluster size and shape can be derived from the numbers $d_k^{\pm}$.

The density functions $d_k^{\pm}$ represent six geometric classes:

(1) isolated points with density $d_4^+ + d_0^-$
(2) cluster corners with density ${}^a d_2^+ + {}^a d_2^-$
(3) cluster edges with density $d_1^+ + d_3^-$
(4) cluster interiors with density $d_0^+ + d_4^-$
(5) protuberances with density $d_3^+ + d_1^-$
(6) bridges with density ${}^0 d_2^+ + {}^0 d_2^-$

We note that any $(-)$ cluster of size above two contains at least one site in its neighborhood with 2 or more $(-)$ neighbors. Since at *very low temperature* (cf. Table I) $d_k \sim 0$ for $k \geqslant 2$, it follows that almost all clusters are isolated and at most of size 2. Since, on the other hand, each $(-)$ doublet contains two $(-)$ protuberances, we infer that, for $\beta \gg \beta_c$, the density of $(-)$ doublets is $(1/2)d_1^-$. An analogous observation holds for $(+)$ singlets and doublets in the negative branch of magnetization.

At *subcritical temperatures*, even close to β_c, d_4 remains quite small, indicating that bulky $(-)$ clusters remain rare in the positive m branch. But as β crosses β_c, (2.4) and (2.5) imply that $(+)$ and $(-)$ clusters become equally probable. *Close to* β_c, the large $d_0 = d_4$ values further indicate that the clusters are quite large. This is characteristic for strong ferromagnetic binding.

As the *supercritical temperature* further increases, the expected $(\pm)$ bulk values $d_0 = d_4$ gradually decrease, indicating a weakening of ferromagnetism, until they reach the values (2.3) at $\beta = 0$. The fact that the boundary term d_2 increases more rapidly with β than either d_1 or d_3, shows that the cluster shapes become more "rugged."

The *antiferromagnetic case* $(J < 0)$ can be obtained by changing β to $-\beta$ in (2.1). Under this substitution the quantities $\varphi, \psi, 1 - s_{01}$ change to $-\varphi, -\psi, 1 + s_{01}$, and a remains unchanged. Since $m \equiv 0$ for all $\beta < \beta_c$, this leads to the symmetries

$$d_k(-\beta) = d_k(\beta), \qquad d_k^{\pm}(-\beta) = d_k^{\mp}(\beta) \tag{3.1}$$

valid in the range $-\beta_c < \beta < \beta_c$. But since m remains zero even for $\beta < -\beta_c$, there are no bifurcations in the antiferromagnetic domain and equations (2.4) and (2.5) hold true at all negative temperatures.

For $\beta \to -\infty$ the mean boundary length $l = 1 - s_{01}$ approaches 2. The corresponding configuration is the checkerboard. At finite negative temperatures $\beta > -\infty$ one expects checkerboard-type configurations with impurities. The d_k values for $\beta < -\beta_c$ are given in Table III. The range $-\beta_c < \beta < 0$ can be covered by applying the symmetries (3.1) to Table I. No discontinuities occur at $-\beta_c$.

Postscript. The reader interested in "testing" our results may consult Ref. 4, where computer simulations of typical equilibrium configurations can be found.

Table III. Equilibrium Expectations of l and d_k (Antiferromagnet)

β	l	d_0	d_1	d_2
−0.45	1.7566	0.3569	0.1127	0.0608
−0.5	1.8728	0.4277	0.0632	0.0182
−0.55	1.9256	0.4587	0.0381	0.0065
−0.6	1.9546	0.4752	0.0235	0.0025
−0.65	1.9716	0.4847	0.0148	0.0010
−0.7	1.9819	0.4904	0.0094	0.0004
−0.75	1.9883	0.4939	0.0060	0.0002
−0.8	1.9924	0.4961	0.0039	0.0001

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