A derivative formula for the free energy function

Yu Zhang

Abstract

We consider bond percolation on the $\mathbb{Z}^d$ lattice. Let $M_n$ be the number of open clusters in $B(n) = [-n, n]^d$. It is well known that $E_p M_n/(2n + 1)^d$ converges to the free energy function $\kappa(p)$ at the zero field. In this paper, we show that $\sigma^2_p(M_n)/(2n + 1)^d$ converges to $-(p^2(1-p)/2 + p(1-p)^2)\kappa'(p)$.

1 Introduction and statement of results.

Consider bond percolation on the $\mathbb{Z}^d$ lattice, in which bonds are independently open with probability $p$ and closed with probability $1-p$. The corresponding probability measure on the configurations of open and closed bonds is denoted by $P_p$. We also denote by $E_p(X)$ and $\sigma^2_p(X)$ the expectation and the variance of $X$ with respect to $P_p$. The open cluster of the vertex $x$, $C(x)$, consists of all vertices that are connected to $x$ by an open path. Here an open path from $u$ to $v$ is a sequence $(v_0,b_0,v_1,...,v_i,b_i,v_{i+1},...,v_n)$ with distinct vertices $v_i$ ($0 \leq i \leq n$) and open bonds $b_i$ adjacent $v_i$ and $v_{i+1}$ such that $v_0 = u$ and $v_n = v$. For vertex set $A$, $A_e$ denotes the bonds with both vertices in $A$. Also, $|A|$ denotes the cardinality of $A$, and $|A_e|$ denotes the number of bonds in $A_e$. We choose $0$ as the origin. The percolation probability is

$$\theta(p) = P_p(|C(0)| = \infty),$$

and the critical probability is

$$p_c = \sup\{p : \theta(p) = 0\}.$$

We denote the open cluster distribution by

$$\theta_n(p) = P_p(|C(0)| = n).$$

By analogy with the Ising model, we introduce the magnetization function as

$$M(p,h) = 1 - \sum_{n=0}^{\infty} \theta_n(p)e^{-nh} \text{ for } h \geq 0.$$

By setting $h = 0$ in the magnetization function,

$$M(p,0) = \theta(p).$$

AMS classification: 60K35.

Key words and phrases: percolation, free energy, variance.
Using term by term differentiation, we also have
\[
\lim_{h \to 0^+} \frac{\partial M(p, h)}{\partial h} = E_p(|C(0)|; |C(0)| < \infty) = \chi(p).
\]

\(\chi(p)\) is called the mean cluster size. The free energy \(F(p, h)\) is defined by
\[
F(p, h) = h(1 - \theta_0(p)) + \sum_{n=1}^{\infty} \frac{1}{n} \theta_n(p) e^{-hn} \text{ for } h > 0.
\]

If we differentiate with respect to \(h\), then we find
\[
\frac{\partial F(p, h)}{\partial h} = M(p, h).
\]

For \(h > 0\), the free energy is infinitely differentiable with respect to \(p\). If \(h = 0\), \(F(p, 0)\) is called the zero-field free energy. The zero-field free energy \(F(p, 0)\) is a more interesting and more difficult object of study since it is believed that there is a singularity point at \(p_c\). By our definition,
\[
F(p, 0) = E(|C(0)|^{-1}; |C(0)| > 0).
\]

Grimmett (1981) discovered that the zero-field free energy also coincides with the number of open clusters per vertex. Let us define the number of open clusters per vertex as follows. We denote by \(M_n\) the number of open clusters in \(B(n)\). By a standard ergodic theorem (see Theorem 4.2 in Grimmett (1989)), the limit
\[
\lim_{n \to \infty} \frac{1}{|B(n)|} M_n = \lim_{n \to \infty} \frac{1}{2(n + 1)^d} M_n = \kappa(p) \text{ a.s. and } L_1
\]
exists for all \(0 \leq p \leq 1\). \(\kappa(p)\) is called the number of open clusters per vertex. Grimmett (1981) proved that
\[
\kappa(p) = F(p, 0).
\]

\(\kappa(p)\), as a function of \(p\), is analytic for \(p \neq p_c\) and differentiable on \([0, 1]\) (see Kesten (1982)). In particular, \(\kappa(p)\) is proved (see Kesten (1982)) to be twice differentiable at \(p_c\) for the square lattice. In general, physicists believe that the zero-field free energy is twice, but not three times differentiable at \(p_c\).

On the other hand, for \(\kappa(p)\), as a limit of random variables, Zhang (2001) showed the following central limit theorem. For \(p \in [0, 1]\),
\[
\frac{M_n - E_p M_n}{\sigma_p(M_n)} \Rightarrow \text{a standard normal distribution.}
\]

Zhang also showed large deviations for \(M_n\). In this paper, we show another property for \(\kappa(p)\).

**Theorem.** For \(0 \leq p \leq 1\),
\[
\lim_{n \to \infty} \sigma_p^2(M_n)/(2n + 1)^d = -(p^2(1-p) + p(1-p)^2)\kappa'(p).
\]
Remark. If \( b_0 \) is the bond with vertices \( 0 \) and \( (1,0,\cdots,0) \), and \( \mathcal{G}(b) \) is the event that there does not exist an open path in \( \mathbb{Z}^d_\epsilon \setminus b \) connecting the two vertices of bond \( b \), then by (2.9) in the proof of the theorem, we have
\[
\kappa'(p) = -dP_p(\mathcal{G}(b_0)).
\] (1.5)

By using Sykes and Essam’s formula (1964), we know that for the square lattice,
\[
\kappa'(0.5) = -1.
\]

Thus
\[
\lim_{n \to \infty} \sigma^2_{0.5}(M_n)/(2n + 1)^d = 0.25.
\] (1.6)

2 Proof of theorem.

For any bond \( b \), let \( v_1(b) \) and \( v_2(b) \) be the two vertices of \( b \). Given \( p \), we start by taking the derivative of \( E_p(M_n) \). Note that
\[
E_p M_n = \sum_{l=1}^{\infty} P_p(M_n \geq l),
\]
and the event \( \{M_n \geq l\} \) is decreasing. Let \( \{M_n \geq l\}(b) \) be the event that \( b \) is a pivotal bond for \( \{M_n \geq l\} \). By Russo’s formula, note that \( P_p(M_n \geq 1) = 1 \), so
\[
\frac{dE_p(M_n)}{dp} = -\sum_{l=2}^{\infty} \sum_{b \in B_e(n)} P_p(\{M_n \geq l\}(b))
\]
\[
= -\sum_{b \in B_e(n)} \sum_{l=2}^{\infty} P_p(M_n = l - 1 \text{ or } l \text{ if } b \text{ is open or closed})
\]
\[
= -\sum_{b \in B_e(n)} P_p \left( \bigcup_{l=2}^{\infty} M_n = l - 1 \text{ or } l \text{ if } b \text{ is open or closed} \right). \tag{2.1}
\]

Let
\[
\mathcal{E}_n(b) = \{ b \text{ is a pivotal bond for the open connection of } v_1(b) \text{ and } v_2(b) \text{ in } B(n) \}.
\]

In other words, if \( b \) is open, then \( v_1(b) \) and \( v_2(b) \) are connected by open paths. Conversely, if \( b \) is closed, then \( v_1(b) \) and \( v_2(b) \) are not connected by open paths. Thus, for each \( b \in B_e(n) \),
\[
P_p \left( \bigcup_{l=2}^{\infty} M_n = l - 1 \text{ or } l \text{ if } b \text{ is open or closed} \right) = P_p(\mathcal{E}_n(b)). \tag{2.2}
\]

Let \( \mathcal{G}_n(b) \) be the event that there does not exist an open path connecting \( v_1(b) \) to \( v_2(b) \) inside \( B_e(n) \setminus b \). Then we would have
\[
\mathcal{E}_n(b) = \mathcal{G}_n(b). \tag{2.3}
\]
Figure 1: The figure shows that $G_n(b)$ occurs, but $G(b)$ does not occur. The two vertices of $b$ are connected by open paths, but they have to reach to the boundary of $B(n)$ before connecting with each other. The dotted path indicates the closed bonds that block the connection of open paths from $v_1(b)$ and $v_2(b)$ inside $B(n)$.

To see (2.3), if there were such a path, then $v_1(b)$ and $v_2(b)$ would always be connected by an open path whenever $b$ is open or closed. So $b$ would not be a pivotal bond. On the other hand, if there does not exist an open path connecting $v_1(b)$ and $v_2(b)$ in $B_e(n) \setminus b$, then $b$ should be a pivotal bond for the open connection of $v_1(b)$ and $v_2(b)$. With these observations,

$$\frac{dE_pM_n}{dp} = - \sum_{b \in B_e(n)} P_p(G_n(b)) = - \sum_{b \in B(n)} P_p(G(b)) - \sum_{b \in B_e(n)} P_p \left( G_n(b) \cap G^c(b) \right).$$

By translation invariance, the ratio of the first term above is

$$\sum_{b \in B_e(n)} P_p(G(b))/|B_e(n)| = P_p(G(b_0)).$$  \hspace{1cm} (2.4)

We use the following lemma to estimate the second term.
Lemma.
\[\lim_{n \to \infty} \frac{1}{|B_e(n)|} \sum_{b \in B_e(n)} P_p \left( \mathcal{G}_n(b) \cap \mathcal{G}^C(b) \right) = 0 \text{ uniformly on } [0, 1].\]

Proof. Let \( A(n, m) = B(n) \setminus B(m) \) for \( m \leq n \), and let \( \bar{A}(n, m) \) be the closure of \( A(n, m) \). Then

\[
\frac{1}{|B_e(n)|} \sum_{b \in B_e(n)} P_p \left( \mathcal{G}_n(b) \cap \mathcal{G}^C(b) \right) \\
\leq \frac{1}{|B_e(n)|} \sum_{b \in B_e(n-\sqrt{n})} P_p \left( \mathcal{G}_n(b) \cap \mathcal{G}^C(b) \right) + \frac{1}{|B_e(n)|} \sum_{b \in A_e(n,n-\sqrt{n})} P_p \left( \mathcal{G}_n(b) \cap \mathcal{G}^C(b) \right) \\
\leq \frac{1}{|B_e(n)|} \sum_{b \in B_e(n-\sqrt{n})} P_p \left( \mathcal{G}_n(b) \cap \mathcal{G}^C(b) \right) + O \left( n^{-0.5} \right),
\]

(2.5)

where we may assume that \( n - \sqrt{n} \) is an integer; otherwise we may use \( \lceil n - \sqrt{n} \rceil \) to replace \( n - \sqrt{n} \).

Let us estimate the first term in the above inequality. For \( b \in B_e(n-\sqrt{n}) \), \( \mathcal{E}_n(b) \cap \mathcal{E}^C(b) \) implies that there exists an open path from \( v_1(b) \) and \( v_2(b) \) without using \( b \), but open paths cannot stay inside \( B(n) \). In other words, the open path adjacent to \( v_1(b) \) has to reach the boundary of \( B(n) \) before reaching \( v_2(b) \) (see Fig. 1). Similarly, the open path adjacent to \( v_2(b) \) has to reach the boundary of \( B(n) \) before reaching \( v_1(b) \) (see Fig. 1). Therefore, there exist two disjoint open paths from \( v_1(b) \) and \( v_2(b) \) such that both reach to the boundary of \( v_1(b) + B(\sqrt{n} - 1) \). Let \( \mathcal{D}(b, \sqrt{n}) \) be the event. By using the estimate of Theorem 6.1 in Grimmett (1989), for all \( p \in [0, 1] \), there exist constant \( C = C(d) \) and \( \delta = \delta(d) \leq 0.5 \) such that

\[ P_p \left( \mathcal{D}(b, \sqrt{n}) \right) \leq C n^{-\delta}. \]

(2.6)

By (2.5) and (2.6),

\[ \frac{1}{|B_e(n)|} \sum_{b \in B_e(n)} P_p \left( \mathcal{G}(b) \cap \mathcal{G}_n^C(b) \right) \leq O(n^{-\delta}). \]

(2.7)

Therefore, the lemma follows from (2.7). \( \square \)

It follows from (2.3), the lemma, and (2.4) that

\[ \frac{dE_p M_n}{|B(n)| dp} = -\left( |B_e(n)|/|B(n)| \right) \sum_{b \in B(n)} P_p(\mathcal{G}(b))/|B_e(n)| + O(n^{-\delta}). \]

(2.8)

Note that

\[ |B_e(n)| = 2dn(2n + 1)^{d-1} \quad \text{and} \quad |B(n)| = (2n + 1)^d, \]

so if we let \( n \to \infty \) in (2.8),

\[ \kappa'(p) = -\lim_{n \to \infty} \sum_{b \in B_e(n)} P_p(\mathcal{G}_n(b))/(2n + 1)^d = -dP_p(\mathcal{G}(b_0)). \]

(2.9)
Now we estimate the variance of $M_n$. We list the bonds in $B_e(n)$ in some order:

$$\{b_1, \cdots, b_k\}.$$  

We define the independent Bernoulli-random variables $\{\omega(b_i)\}$ for $1 \leq i \leq k$ to be $\omega(b_i) = 0$ (open) or $\omega(b_i) = 1$ (closed) with probability $p$ or $1 - p$. Now we construct the following filtration:

$$\mathcal{F}_0 = \{\emptyset, \Omega\} \subset \mathcal{F}_1 = \{\sigma\text–field generated by } \omega(e_1)\} \subset \cdots \subset \mathcal{F}_k = \{\sigma\text–field generated by } \omega(e_1), \cdots, \omega(e_k)\}.$$  

The martingale representation of $M_n - \mathbb{E}_\rho M_n$ is

$$M_n - \mathbb{E}_\rho M_n = \sum_{i=0}^{k-1} [\mathbb{E}_\rho(M_n|\mathcal{F}_{i+1}) - \mathbb{E}_\rho(M_n|\mathcal{F}_i)].$$  

Let the martingale difference be

$$\Delta_{i,k} = [\mathbb{E}_\rho(M_n|\mathcal{F}_{i+1}) - \mathbb{E}_\rho(M_n|\mathcal{F}_i)].$$  

The variance is

$$\sigma^2_{\rho}(M_n) = \sum_{i=0}^{k-1} \mathbb{E}_\rho(\Delta_{i,k}^2). \quad (2.10)$$  

Both $M_n$ and $\Delta_{i,k}$ can be viewed as functions on $[0, 1]^k$ and $[0, 1]^i$, respectively. So we can write $M_n(c_1, \cdots, c_k)$ and $\Delta_{i,k}(c_1, \cdots, c_i)$ for them, where $c_i$ only takes a value of zero or one. Thus

$$\Delta_{i,k} = \Delta_{i,k}(c_1, \cdots, c_i)$$

$$= \sum_{c_{i+1}, \cdots, c_k} M_n(c_1, \cdots, c_{i+1}, \cdots, c_k) \mathbb{P}_\rho (\omega(b_{i+1}) = c_{i+1}, \cdots, \omega(b_k) = c_k)$$

$$- \sum_{c'_i, c_{i+1}, \cdots, c_k} M_n(c_1, \cdots, c_{i-1}, c'_i, c_{i+1}, \cdots, c_k) \mathbb{P}_\rho (\omega(b_i) = c'_i, \omega(b_{i+1}) = c_{i+1}, \cdots, \omega(b_k) = c_k)$$

$$= \sum_{c'_i, c_{i+1}, \cdots, c_k} [M_n(c_1, \cdots, c_i, c_{i+1}, \cdots, c_k) - M_n(c_1, \cdots, c_{i-1}, c'_i, c_{i+1}, \cdots, c_k)]$$

$$\cdot \mathbb{P}_\rho (\omega(b_i) = c'_i, \omega(b_{i+1}) = c_{i+1}, \cdots, \omega(b_k) = c_k), \quad (2.11)$$

where the sum takes over all possible values of $c_i$ and $c'_i$. On $\mathcal{G}_n^C(b_i)$,

$$M_n(c_{i+1}, \cdots, c_i, \cdots, c_k) - M_n(c_{i+1}, \cdots, c'_i, 0, \cdots, c_k) = 0 \text { for } c_i = 0 \text { or } c_i = 1,$$

$$M_n(c_{i+1}, \cdots, c_i, \cdots, c_k) - M_n(c_{i+1}, \cdots, 1, \cdots, c_k) = 0 \text { for } c_i = 0 \text { or } c_i = 1.$$

Thus, by (2.11),

$$\Delta_{i,k} \left(1 - I_{\mathcal{G}_n(b_i)} \right) = 0, \quad (2.12)$$

where $I_A$ is the indicator of $A$. With this observation,

$$\Delta_{i,k} = \Delta_{i,k} I_{\mathcal{G}_n(b_i)}. \quad (2.13)$$
Note that on $\mathcal{G}_n(b_i)$,

$$[M_n(c_1, \cdots, c_i = 1, \cdots, c_k) - M_n(c_1, \cdots, c_{i-1}, c_i' = 0, c_{i+1}, \cdots, c_k)] = -1.$$ 

so

$$\Delta_{i,k}(c_1, \cdots, c_{i-1}, 1) I_{\mathcal{G}_n(b_i)}$$

\begin{align*}
&= I_{\mathcal{G}_n(b_i)} \sum_{c_{i+1}, \cdots, c_k} [M_n(c_1, \cdots, c_i = 1, \cdots, c_k) - M_n(c_1, \cdots, c_{i-1}, c_i' = 0, c_{i+1}, \cdots, c_k)] \\
&\quad \cdot P_p(\omega(b_{i+1}) = c_{i+1}, \cdots, \omega(b_k) = c_k) \\
&\quad + I_{\mathcal{G}_n(b_i)} \sum_{c_{i+1}, \cdots, c_k} [M_n(c_1, \cdots, c_i = 1, \cdots, c_k) - M_n(c_1, \cdots, c_{i-1}, c_i' = 1, c_{i+1}, \cdots, c_k)] \\
&\quad \cdot P_p(\omega(b_{i+1}) = c_{i+1}, \cdots, \omega(b_k) = c_k) \\
&\quad - (1 - p) I_{\mathcal{G}_n(b_i)} \\
&= (1 - p)^2 I_{\mathcal{G}_n(b_i)}. \\
\end{align*}

Therefore,

$$\Delta_{i,k}(c_1, \cdots, c_{i-1}, 1) I_{\mathcal{G}_n(b_i)} = (1 - p)^2 I_{\mathcal{G}_n(b_i)}.$$ 

(2.14)

Similarly, note that on $\mathcal{G}_n(b_i)$,

$$[M_n(c_1, \cdots, c_i = 0, \cdots, c_k) - M_n(c_1, \cdots, c_{i-1}, c_i' = 1, c_{i+1}, \cdots, c_k)] = 1.$$ 

so

$$\Delta_{i,k}(c_1, \cdots, c_{i-1}, 0) I_{\mathcal{G}_n(b_i)}$$

\begin{align*}
&= I_{\mathcal{G}_n(b_i)} \sum_{c_{i+1}, \cdots, c_k} [M_n(c_1, \cdots, c_i = 0, \cdots, c_k) - M_n(c_1, \cdots, c_{i-1}, c_i' = 0, c_{i+1}, \cdots, c_k)] \\
&\quad \cdot P_p(\omega(b_{i+1}) = c_{i+1}, \cdots, \omega(b_k) = c_k) \\
&\quad + I_{\mathcal{G}_n(b_i)} \sum_{c_{i+1}, \cdots, c_k} [M_n(c_1, \cdots, c_i = 0, \cdots, c_k) - M_n(c_1, \cdots, c_{i-1}, c_i' = 1, c_{i+1}, \cdots, c_k)] \\
&\quad \cdot P_p(\omega(b_{i+1}) = c_{i+1}, \cdots, \omega(b_k) = c_k) \\
&\quad - p I_{\mathcal{G}_n(b_i)} \\
&= p^2 I_{\mathcal{G}_n(b_i)} \\
\end{align*}

Therefore,

$$\Delta_{i,k}(c_1, \cdots, c_{i-1}, 0) I_{\mathcal{G}_n(b_i)} = p^2 I_{\mathcal{G}_n(b_i)}.$$ 

(2.15)
Together with (2.13), (2.14) and (2.15),

\[ E_p \Delta_{i,k}^2 = E_p \Delta_{i,k}^2 I_{G_n(b_i)} = E_p \Delta_{i,k}^2(c_1, \ldots, c_{i-1}, 1)I_{\{\omega(b_i)=1\}}I_{G_n(b_i)} + E_p \Delta_{i,k}^2(c_1, \ldots, c_{i-1}, 0)I_{\{\omega(b_i)=0\}}I_{G_n(b_i)} = E_p (1-p)^2 I_{\{\omega(b_i)=1\}}I_{G_n(b_i)} + E_p p^2 I_{\{\omega(b_i)=0\}}I_{G_n(b_i)}. \]

Note that \( \{\omega(b_i)\} \) and \( I_{G_n(b_i)} \) are independent, so

\[ E_p \Delta_{i,k}^2 = [(1-p)^2 p + p^2 (1-p)]E_p I_{G_n(b_i)} = [(1-p)^2 p + p^2 (1-p)]P_p(G_n(b_i)). \] (2.16)

By (2.10) and (2.16),

\[ \sigma^2_p(M_n) = \sum_{i=1}^{k} E_p(\Delta_{i,k}^2) = [(1-p)^2 p + p^2 (1-p)] \sum_{b \in B_e(n)} P_p(G_n(b)). \] (2.17)

Therefore, if we divide the both sides of (2.17) by \((2n+1)^d\) and let \(n\) go to infinity, by (2.9),

\[ \lim_{n \to \infty} \frac{\sigma^2_p(M_n)}{(2n+1)^d} = \lim_{n \to \infty} \frac{[(1-p)^2 p + p^2 (1-p)] \sum_{b \in B_e(n)} P_p(G_n(b))}{(2n+1)^d} = -(1-p)^2 p + p^2 (1-p) \kappa'(p). \]

So the theorem follows.

References

Grimmett, G. (1981). On the differentiability of the number of clusters per vertex in the percolation model. J. Lond. Math. Soc. 23 372–384.

Grimmett, G. (1989). Percolation. Springer-Verlag, New York.

Kesten, H. (1982). Percolation Theory for Mathematicians. Birkhauser, Boston.

Sykes, M. F., and Essam, J. W. (1964). Exact critical percolation probabilities for site and bond problems in two dimensions. J. Math. Phys. 5 1117-1127.

Zhang, Y. (2001). A martingale approach in the study of percolation clusters on the \(Z^d\) lattice. J. Theore. Probab. 14 165–187.

Yu Zhang

Department of Mathematics
University of Colorado
Colorado Springs, CO 80933
yzhang3@uccs.edu