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# Simulating phase transition phenomena of the unitary cell model[†]

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**Abstract**

Lattice process models are used to explain phase transitions in statistical mechanics, a branch of physics. The Ising model, a specific form of lattice process model, was proposed by Ising in 1925. Since then, variants of the Ising model such as the Potts model and the unitary cell model have been proposed. Like the Ising model, it is believed that the more general models exhibit phase transitions on the critical surface, which is based on the mathematical equation. In statistical sense, phase transitions can be simulated through Markov Chain Monte Carlo (MCMC). We applied Swendsen-Wang algorithm, a block Gibbs algorithm, to a general lattice process models and we simulate phase transition phenomena of the unitary cell model.

*Keywords*: Critical surface, phase transition, Swendsen-Wang algorithm, unitary cell model.

## 1. Introduction

The Ising model was originally introduced in statistical mechanics to describe macroscopic properties of a mechanical system which is made up of a large number of molecules. Typical examples include a gas, a fluid or a magnet. Ever since the Ising model was proposed by Ising in 1925, variants of the Ising model have been proposed such as the Potts model (Potts, 1952) and the unitary cell model (Aguilar and Braun, 1991a; Aguilar and Braun, 1991b). Like the Ising model, it is believed that the more general models exhibit phase transitions on the critical surface.

Lattice process models also have potential for fitting spatial data on a lattice and for explaining spatial interaction between variables. For example, lattice process models may provide modeling for plant ecology data (Besag, 1974; Cressie, 1993) and Bayesian image restoration (Geman and Geman, 1984).

However, it is not clear how lattice process models explain complex phenomena, or why the various interesting patterns emerge suddenly near the critical value. The first step to answer above questions is to generate realizations from the lattice model near the critical

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surface and investigate whether the pattern of the realization of the lattice process models is abruptly changed. The inference for spatial data can be also made through the simulation.

Statistical analysis for lattice process models has problems for generation of realizations, estimation or test since an exact probability density for lattice process models is unavailable. However, the developments in Markov Chain Monte Carlo (MCMC) make it possible to perform these procedures (Begum and Ali, 2004; Lee, 2004). Kim (2000) applied Swendsen-Wang algorithm, a block Gibbs algorithm, to the general lattice process models. In this paper, we focus on investigating the phase transition of a unitary cell model by the generation of realizations.

This paper is organized as follows. Section 2 introduces the unitary cell model. We explain phase transition in Section 3. In Section 4, we apply the Swendsen-Wang algorithm to the unitary cell model to verify its capability for representing phase transition. Concluding remarks are addressed in Section 5.

## 2. The unitary cell model

The Ising model is used to describe spatial interactions between variables on two-dimensional square lattice. The Ising model exhibits abrupt qualitative changes in behavior at a parameter value called critical value. This property, called phase transition in statistical mechanics, makes the Ising model interesting in physics. There are several lattice process models that are variants of the Ising model. These models have different lattice shapes or include arbitrary interactions between variables or allow the variables to take more than two values. Potts (1952) generalized the Ising model by allowing the variables to take more than two values. Aguilar and Braun (1991a; 1991b) proposed what they called a "unitary cell model". Their model is noteworthy in that various kinds of models are obtained by transforming the shape of the lattice and defining interactions properly. These models are defined by an unnormalized density. MCMC makes it possible to get the realization from this kind of model and to investigate the property of the model.

A unitary cell is made up of variables on $q \times t$ small lattice with arbitrary nearest-neighbor interactions between them. The unitary cell is repeated $m \times n$ times. For visualization, the lattice is usually depicted like a checkerboard. Figure 2.1 shows the $2 \times 2$ unitary cell lattice, which means the size of the unitary cell is $2 \times 2$. Each circle is called a vertex or site and a random variable taking only two values, resides on each vertex. The vertices are joined by "edges" and there exists interaction along the edge. Translates of a unitary cell have the same parameter values. Thus, there are as many parameters as there are interactions within a unitary cell. This model has 8 different interaction parameters. The parameters $\theta$ and $\gamma$ represent horizontal and vertical interactions respectively. For the notational convenience, the index $ij$ is used for vertices and $X_{ij}$ is the random variable on vertex $ij$. A density of $q \times t$ unitary cell model is defined as follows.

**Definition 2.1** Let $X_{ij}$ be random variables taking values in $\{-1, 1\}$. Let $\theta_{[i][j]}$ be horizontal interactions between $X_{ij}$ and $X_{i(j+1)}$ and let $\gamma_{[i][j]}$ be vertical interactions between $X_{ij}$ and $X_{(i+1)j}$, $[i] = i \ (mod\ q)$, $[j] = j \ (mod\ t)$. With the lattice size of $mq \times nt$, the

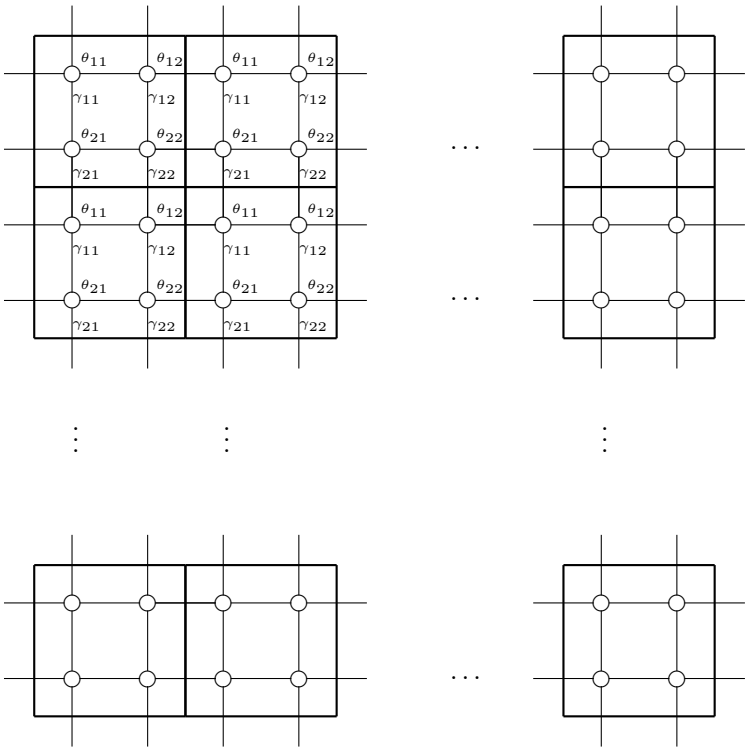



**Figure 2.1** $2 \times 2$ Unitary cell lattice

unnormalized density of the unitary cell model is defined by

$$h(x) = \exp\left(\sum_{i,\ j} \theta_{[i][j]} x_{ij} x_{i(j+1)} \ + \ \gamma_{[i][j]} x_{ij} x_{(i+1)j}\right), \tag{2.1}$$

where $i = 1, \ldots, mq$ and $j = 1, \ldots, nt$. And the normalizing constant is given by

$$c_{m,n}(\theta, \gamma) = \sum_{x} \exp\left(\sum_{i,\ j} \theta_{[i][j]} x_{ij} x_{i(j+1)} \ + \ \gamma_{[i][j]} x_{ij} x_{(i+1)j}\right).$$

## 3. Phase transitions and critical values

A phase transition is the phenomenon in which the probabilities of a lattice process model change abruptly at some parameter value. This models physical phase transitions, such as freezing and boiling of water. Such a parameter value is called the critical value. When the phase transition occurs on the set of parameters, the set is called the critical surface. In this section, we illustrate a phase transition from the known critical value of the Ising model and introduce the critical surface of the unitary cell model. Aguilar and Braun (1991a;

1991b) proposed methods to calculate the normalizing constant and the critical surface of the unitary cell model.

### 3.1. Critical value of the Ising model

Consider random variables on vertex in a lattice having $m$ rows and $n$ columns. Each random variable takes only two values 1 and $-1$. The one-parameter Ising model on an $m \times n$ lattice is defined by unnormalized exponential density

$$h(x) = \exp\Big(\beta\ t_2(x)\Big), \quad \beta \in \mathbb{R}, \tag{3.1}$$

where

$$t_2(x) = \sum_{i \sim j} \mathrm{I}(x_i, x_j)$$

where $\sim$ means neighbor and $\mathrm{I}(\cdot,\cdot)$ is an indicator function. The normalizing constant is

$$c_{m,n}(\beta) = \sum_x \exp\Big(\beta\ t_2(x)\Big).$$

It turns out that calculating the normalizing constant is extremely difficult. Asymptotic characterization of the normalizing constant plays crucial role to explain phase transition mathematically. The limit of the logarithm of the normalizing constant scaled by the lattice size was calculated by Onsager in 1944 (Baxter, 1982). The critical value of the Ising model is $0.5 \sinh^{-1}(1)$. Figure 3.1 shows realizations of the one-parameter Ising model with different parameter values on $256 \times 256$ lattice. Far above the critical value, most of the pixels are black or white in the third row of Figure 3.1 whereas far below the critical value, black and white pixels are mixed about half and half in the first row of Figure 3.1. Near the critical value, a small cluster of black or white is observed as in the second row of Figure 3.1. Note that as the parameter value moves through the critical value, the feature of realization is changed from random pattern to deterministic pattern. An abrupt changes of the feature of the realization occur suddenly as the parameter value passes through the critical value. Only near the critical value, we observe interesting patterns, and far below and far above the critical value, the patterns of the realizations are simple.

### 3.2. Critical surface for the $2 \times 2$ unitary cell model

Aguilar and Braun (1991a) characterized the logarithm of the normalizing constant for the unitary cell model asymptotically as the lattice size goes to infinity, that is, $(m,n) \to \infty$. It turns out that the asymptotic behavior depends on the interaction parameters and derives the critical surface. Following are the asymptotics of logarithm of the normalizing constant, which are equation (30) and equation (31) in Aguilar and Braun (1991a),

$$L(\boldsymbol{\theta}, \boldsymbol{\gamma}) = \lim_{(n,m)\to\infty} \frac{\ln c_{n,m}(\boldsymbol{\theta}, \boldsymbol{\gamma})}{mqnt} = \frac{1}{32\pi^2} \int_0^{2\pi} dx \int_0^{2\pi} dy \ln[32F(\boldsymbol{\theta}, \boldsymbol{\gamma}, x, y)],$$

where

$$
\begin{aligned}
F(\boldsymbol{\theta},\boldsymbol{\gamma},x,y) &= H_1\cos^2(x+y)+H_2\cos^2(x-y)+H_3\cos(x-y)\\
&\quad +H_4\cos(x+y)+H_5\cos^2(x)+H_6\cos(y)+H_7,\\
H_1 &= 2a_{11}a_{12}a_{21}a_{22},\\
H_2 &= 2s_{11}s_{12}s_{21}s_{22},\\
H_3 &= -(b_{11}b_{22}+b_{12}b_{21})(s_{11}s_{12}+s_{21}s_{22})\\
&\quad -(a_{11}a_{12}+a_{21}a_{22})(c_{11}s_{12}s_{21}c_{22}+s_{11}c_{12}c_{21}s_{22})\\
&\quad -(b_{11}b_{12}+b_{21}b_{22})(c_{11}c_{12}s_{21}s_{22}+s_{11}s_{12}c_{21}c_{22}),\\
H_4 &= -(b_{11}a_{12}b_{21}a_{22}+a_{11}b_{12}a_{21}b_{22})(c_{11}c_{21}+c_{12}c_{22})\\
&\quad -(a_{11}a_{21}+a_{12}a_{22})(c_{11}c_{22}+c_{12}c_{21})\\
&\quad -(b_{11}a_{12}a_{21}b_{22}+a_{11}b_{12}b_{21}a_{22})(s_{11}s_{21}+s_{12}s_{22}),\\
H_5 &= -2(s_{12}s_{21}a_{12}a_{21}+s_{11}s_{22}a_{11}a_{22}),\\
H_6 &= -2(s_{12}s_{21}a_{11}a_{22}+s_{11}s_{22}a_{12}a_{21}),\\
H_7 &= 1+c_{11}c_{12}c_{21}c_{22}-s_{11}s_{12}s_{21}s_{22}\\
&\quad +b_{11}b_{12}b_{21}b_{22}(1+c_{11}c_{12}c_{21}c_{22}+s_{11}s_{12}s_{21}s_{22})\\
&\quad +a_{11}a_{12}a_{21}a_{22}(-1+c_{11}c_{12}c_{21}c_{22}+s_{11}s_{12}s_{21}s_{22})\\
&\quad +(b_{11}b_{21}+b_{12}b_{22})(c_{11}c_{12}+c_{21}c_{22})\\
&\quad +(b_{11}b_{12}a_{21}a_{22}+a_{11}a_{12}b_{21}b_{22})(s_{11}c_{12}s_{21}c_{22}+c_{11}s_{12}c_{21}s_{22})\\
&\quad +(s_{12}s_{21}+s_{11}s_{22})(a_{12}a_{21}+a_{11}a_{22})
\end{aligned}
$$

and

$$c_{ij}=\cosh(2\theta_{ij}),\quad s_{ij}=\sinh(2\theta_{ij}),\quad a_{ij}=\sinh(2\gamma_{ij}),\quad b_{ij}=\cosh(2\gamma_{ij}).$$

Aguilar and Braun (1991b) also shows that critical value or critical surface is the set of $(\boldsymbol{\theta},\boldsymbol{\gamma})$ satisfying the equation $v(\boldsymbol{\theta},\boldsymbol{\gamma})=F(\boldsymbol{\theta},\boldsymbol{\gamma},0,0)=0$. That is, critical surface is the set of parameters satisfying following equation, called the critical equation (Aguilar and Braun, 1991b, equation (24)).

$$
\begin{aligned}
v(\boldsymbol{\theta},\boldsymbol{\gamma}) &= (1+c_{11}c_{12}c_{21}c_{22}+s_{11}s_{12}s_{21}s_{22})(1+a_{11}a_{12}a_{21}a_{22}+b_{11}b_{12}b_{21}b_{22})\\
&\quad -(b_{11}b_{12}+b_{21}b_{22})(c_{11}c_{12}s_{21}s_{22}+s_{11}s_{12}c_{21}c_{22})\\
&\quad -(a_{12}a_{21}+a_{11}a_{22})(s_{12}s_{21}+s_{11}s_{22})\\
&\quad +(b_{11}b_{21}+b_{12}b_{22})(c_{11}c_{12}+c_{21}c_{22})\\
&\quad -(a_{11}a_{12}+a_{21}a_{22})(c_{11}s_{12}s_{21}c_{22}+s_{11}c_{12}c_{21}s_{22})\\
&\quad -(b_{11}b_{22}+b_{12}b_{21})(s_{11}s_{12}+s_{21}s_{22})\\
&\quad -(s_{11}s_{21}+s_{12}s_{22})(b_{11}a_{12}a_{21}b_{22}+a_{11}b_{12}b_{21}a_{22})\\
&\quad -(b_{11}a_{12}b_{21}a_{22}+a_{11}b_{12}a_{21}b_{22})(c_{11}c_{21}+c_{12}c_{22})\\
&\quad -(a_{11}a_{21}+a_{12}a_{22})(c_{11}c_{12}+c_{12}c_{21})\\
&\quad +(b_{11}b_{12}a_{21}a_{22}+a_{11}a_{12}b_{21}b_{22})(s_{11}c_{12}s_{21}c_{22}+c_{11}s_{12}c_{21}s_{22})\\
&= 0.
\end{aligned}
\tag{3.2}
$$

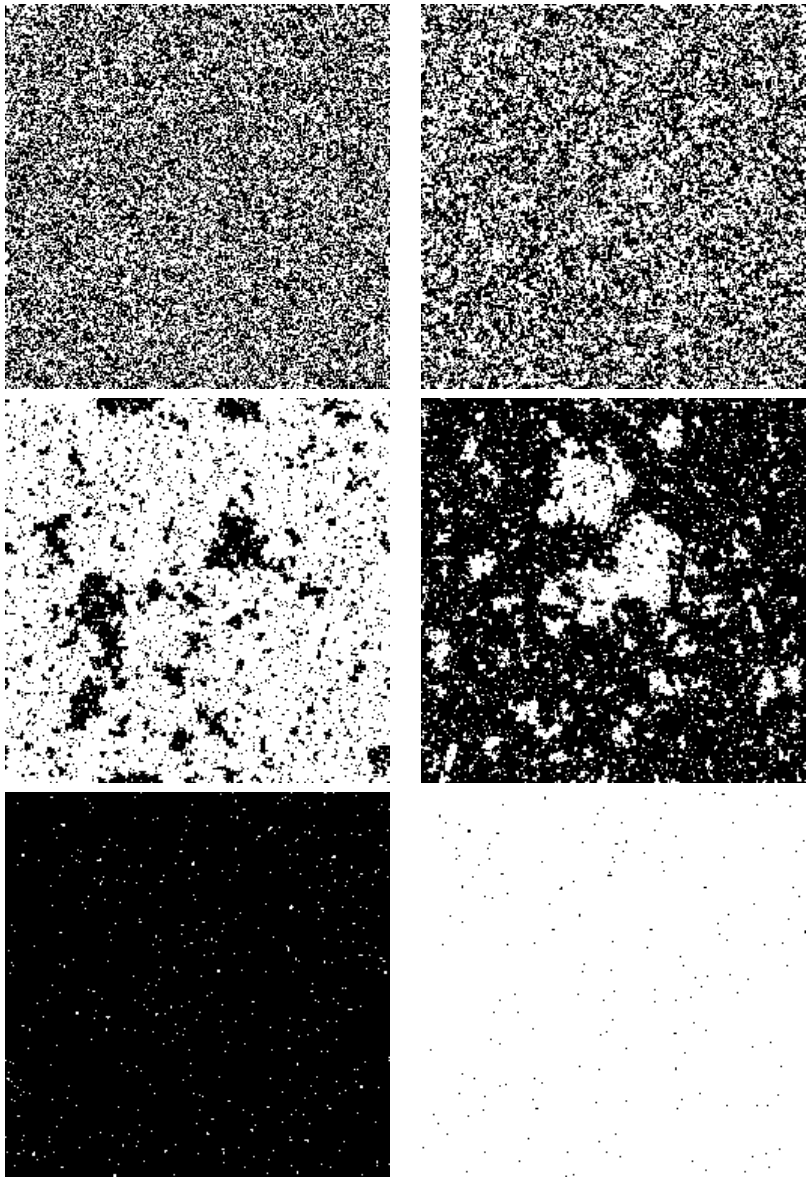


**Figure 3.1** Realizations of $256 \times 256$ one-parameter Ising model with canonical parameter 0.1406868, 0.2406868, 0.4406868, 0.4406868, 0.6406868 and 0.7406868

This equation gives the same critical value for models already solved. For the one-parameter Ising model (equation (3.1)), by setting $\beta = \theta_{ij} = \gamma_{ij}$, and $c = c_{ij} = b_{ij} = \cosh(2\beta)$, $s = s_{ij} = a_{ij} = \sinh(2\beta)$, $i = 1, 2,\ j = 1, 2$, equation (3.2) becomes

$$v(\beta) = 8(s^4 - 1)^2 = 0.$$

Thus, critical value is $0.5\sinh^{-1}(1)$.

## 4. The Swendsen-Wang algorithm and case study

A realization of lattice process model can be obtained by MCMC, although mixing rate is slow. Swendsen and Wang (1987) introduced so-called auxiliary variables (Besag and Green, 1993) to speed up the mixing of the Potts model. Potts (1952) generalized the Ising model by allowing the variables to take $q$ distinct values. The Potts model used as a model for images with $q$ colors. The state of a variable is called "color" and state of all the variables represents an image. Potts considered nearest-neighbor interactions on square lattices. Let $L_{m\times n}$ be a two-dimensional lattice and let $Q$ be a set of $q$ distinct values, say $Q = \{1, 2, \ldots, q\}$. The state space $S$ of the Potts model is the set

$$S = Q^{L_{m\times n}}.$$

The Potts model allows one to define interactions between vertices, say $1, 2, \ldots, N$. These interactions depend only on whether two vertices have the same value or same color. The unnormalized density of the Potts model is

$$h(y) = \exp\Big(Q_1(\alpha; y) + Q_2(\beta; y)\Big),$$

where

$$Q_1(\alpha; y) = \sum_i \alpha_i(y_i),\ \alpha_i \text{ is a real-valued function from } Q,$$
$$Q_2(\beta; y) = \sum_{i\sim j} \beta_{ij}\mathrm{I}(y_i, y_j),$$

and

$$\mathrm{I}(y_i, y_j) = \begin{cases} 1 & \text{if } y_i = y_j \text{ for i, j = 1, 2, \ldots, N} \\ 0 & \text{else.} \end{cases}$$

Usually, $\beta_{ij}$ is defined as depending on the distance between vertices, i.e. equal distance implies equal $\beta_{ij}$.

Auxiliary variables $Z_{ij}$, called bonds, are added between vertices, i.e. each pair of vertices $i$ and $j$ gets "bond" variable $Z_{ij}$. But if the interaction term $\beta_{ij}$ is 0, then the bond variable is omitted. The $Z_{ij}$ take values in $\{0, 1\}$. Thus, the extended state space $S^e$ is

$$S^e = Q^{L_{m\times n}} \times \{0, 1\}^{L_{m\times n}\times L_{m\times n} - L'_{m\times n}},$$

where $L_{m\times n}$ is the $m \times n$ lattice and $L'_{m\times n}$ is the set $\{\,(i, i) : i \in L_{m\times n}\,\}$.

The unnormalized joint distribution of an image $Y$ and bonds $Z$ is constructed by specifying the conditional distribution of bonds $Z$ given the image $Y$ so that the marginal distribution of $Y$ is the Potts model. The conditional distribution of $Z_{ij}$ given $Y$ is defined by

$$\begin{aligned} f(z_{ij}|y) &= \begin{cases} p_{ij}^{z_{ij}}(1 - p_{ij})^{(1-z_{ij})}, & \text{if } y_i = y_j \\ 1 - z_{ij}, & \text{if } y_i \neq y_j \end{cases} \\ &= p_{ij}^{z_{ij}}(1 - p_{ij})^{(1-z_{ij})}\mathrm{I}(y_i, y_j) + (1 - z_{ij})\,(1 - \mathrm{I}(y_i, y_j)) \end{aligned}$$

where $p_{ij} = 1 - \exp(-\beta_{ij})$.

When $Z_{ij} = 1$, vertices $i$ and $j$ are said to be bonded. The conditional distribution of $Z_{ij}$ given $Y$ indicates that two vertices cannot be bonded when $Y_i \neq Y_j$. Thus, variables on the bounded vertices must have the same value. The bonds are conditionally independent given the image $Y$. Thus, the conditional distribution of $Z$ given $Y$ is

$$f(z|y) = \prod_{i \neq j} \left\{ p_{ij}^{z_{ij}} (1 - p_{ij})^{(1-z_{ij})} \mathrm{I}(y_i, y_j) + (1 - z_{ij}) \left(1 - \mathrm{I}(y_i, y_j)\right) \right\}.$$

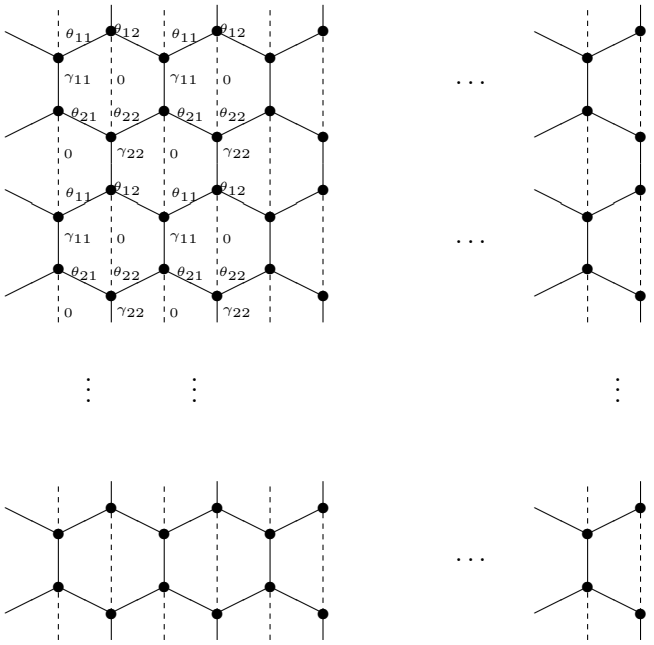
Note that equivalence relation $*$ on $L \times L$ ($L = L_{m \times n}$) can be defined as $i * j$ if and only if $Z_{ij} = 1$. This equivalence relation $*$ partitions the lattice $L$ into subsets, say, $L_1, L_2, \ldots, L_r$ for some finite $r$. Call each $L_k, k = 1, \ldots, r$, a cluster. If vertices $i$ and $j$ belongs to the same cluster, then the bond variable $Z_{ij} = 1$. Otherwise, $Z_{ij} = 0$. The unnormalized conditional distribution of $Y$ given $Z$ is proportional to the unnormalized joint distribution and the parts, not a function of $y$ can be ignored. Hence,

$$\begin{aligned} h(y|z) \propto h(y, z) &= \exp\Big( Q_1(\alpha; y) + Q_2(\beta; y) \Big) \\ &\quad \times \prod_{i \neq j} \left\{ p_{ij}^{z_{ij}} (1 - p_{ij})^{(1-z_{ij})} \mathrm{I}(y_i, y_j) + (1 - z_{ij}) \left(1 - \mathrm{I}(y_i, y_j)\right) \right\} \\ &\propto \left\{ \prod_{k=1}^{r} \exp\left( \sum_{i \in L_k} \alpha_i(y_i) \right) \right\}. \end{aligned}$$

The choice $p_{ij} = 1 - \exp(-\beta_{ij})$ makes the clusters independent given the bonds. Thus, the state of each cluster given the bonds can be updated independently. The image variables in the same cluster are updated at the same time. Since image variables in the same cluster are bonded, those variables must all have the same color. The Swendsen-Wang algorithm uses the so-called block Gibbs update, that is, updates images given bonds and then updates bonds given images. The image variable is a realization from the Potts model.

Swendsen-Wang algorithm, a block Gibbs algorithm, can be applied to the $2 \times 2$ unitary cell model since the unitary cell model is the special case of the Potts model. The $2 \times 2$ unitary cell model is especially interesting in the sense that it includes the Ising model, the triangular lattice model, the hexagonal lattice model, etc. By transforming the shape of the unitary cell and manipulating the interaction terms, any of these models can be obtained. For example, consider the general hexagonal lattice model which has 6 interaction parameters on the hexagonal lattice. If we transform the shape of the square cell to the hexagonal form and set interaction terms $\gamma_{12} = \gamma_{21} = 0$ in Figure 2.1, then the general hexagonal lattice model is obtained. Note that since interaction terms $\gamma_{12}$ and $\gamma_{21}$ in the model (2.1) are zero, there is no interaction along the corresponding edges. The resulting model has two different kinds of interaction pattern on hexagonal cell and these patterns are repeated over the whole lattice. The top panel and bottom panel of Figure 4.1 describe the general hexagonal lattice and its two different patterns of interaction, respectively.

The hexagonal lattice model can be used to explore the properties of a mechanical system such as crystal or snowflake as the Ising model was originally proposed as a model for magnetization of a magnet. For illustration, we will investigate the phase transition of a




Two Different Hexagons

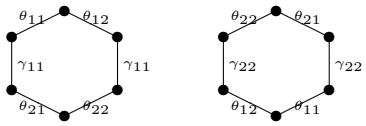



**Figure 4.1** Lattice of the general hexagonal model

symmetric hexagonal lattice model through generation of realizations by Swendsen-Wang algorithm in statistical sense. Let $c_{ij} = \cosh(2\theta_{ij})$, $s_{ij} = \sinh(2\theta_{ij})$, $a_{ij} = \sinh(2\gamma_{ij})$ and $b_{ij} = \cosh(2\gamma_{ij})$ for the general hexagonal lattice model having six interaction parameters. Since $\gamma_{12} = \gamma_{21} = 0$, $a_{12} = a_{21} = 0$ and $b_{12} = b_{21} = 1$, the critical equation (3.2) is simplified as

$$\begin{aligned} & v(\boldsymbol{\theta}, \gamma_{11}, \gamma_{22}) \\ &= (s_{11} + s_{12})(s_{21} + s_{22})(b_{11}b_{22} + 1) - a_{11}a_{22}(s_{11}s_{12} - 1)(s_{21}s_{22} - 1) \\ &\quad - a_{11}a_{22}c_{11}c_{12}c_{21}c_{22} \\ &= 0. \end{aligned}$$

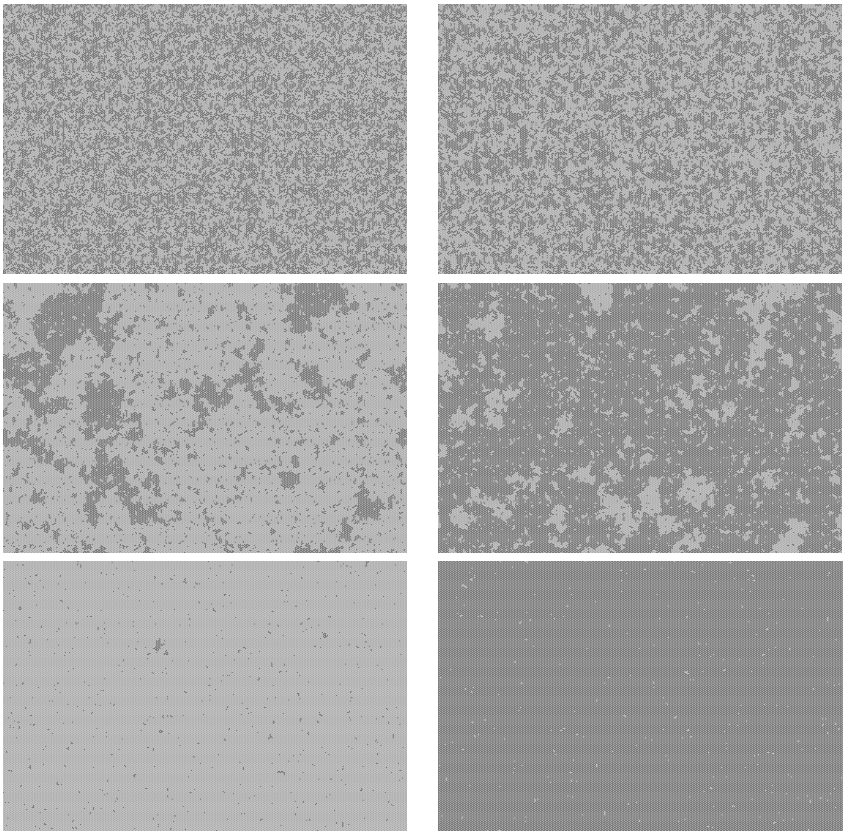


**Figure 4.2** Realizations of the symmetric hexagonal lattice model at parameter value $\beta_c - 0.3$, $\beta_c - 0.2$, $\beta_c$, $\beta_c$, $\beta_c + 0.2$ and $\beta_c + 0.3$ with lattice size of $256 \times 256$

For a symmetric hexagonal lattice model, all six parameters are equal, say $\beta$. Then

$$v(\beta) = -2s^2(s^2 - 3)(s^2 + 1) = 0,$$

where $s = \sinh(2\beta)$ and $c = \cosh(2\beta)$. So, the critical value $\beta_c$ is

$$\beta_c = \left(\sinh^{-1}(\sqrt{3})/2, \ldots, \sinh^{-1}(\sqrt{3})/2\right).$$

Figure 4.2 illustrates realizations of the symmetric hexagonal lattice model at different parameter values by Swendsen-Wang algorithm. The black and white pixels are randomly distributed far below the critical values $\beta_c - 0.3$ and $\beta_c - 0.2$ in the top panel of Figure 4.2 whereas most of the pixels are black or white far above the critical values $\beta_c + 0.2$ and $\beta_c + 0.3$ in the bottom panel of Figure 4.2. Like the Ising model, small clusters of black or white are spread-out over the lattice at critical value in the middle panel of Figure 4.2. The symmetric hexagonal lattice model also exhibits abrupt qualitative changes in behavior at critical value. Thus this model also has potential for explaining the macroscopic properties of a physical system.

## 5. Concluding remarks

Lattice process models are used to explain phase transitions in statistical mechanics. Although it is believed that the lattice process models exhibit phase transitions satisfying a mathematical equation called the critical surface, we need to verify that the realization of the lattice process model represents the abrupt quality changes near the critical surface. Swendsen-Wang algorithm, a block Gibbs algorithm, makes it possible to generate a realization from an unnormalized lattice process model. We investigate the phase transitions of a symmetric hexagonal lattice model through a case study using Swendsen-Wang algorithm and conform that this kind of model has a potential for explaining the macroscopic properties of a physical system.

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