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NUMERICAL STUDY OF THE 6-VERTEX MODEL WITH DOMAIN WALL BOUNDARY CONDITIONS

by David ALLISON (*) & Nicolai RESHETIKHIN (**)

Introduction.

It is well known that the 6-vertex model with periodical boundary conditions has phase transitions. The history and the classification of phases in the 6-vertex model as well as many interesting facts about the structure of the partition function of the 6-vertex model with periodic boundary conditions can be found in [10], [3]. The 6-vertex model is solvable in the sense that row-to-row transformations can be diagonalized by the Bethe ansatz. These transformations form a commutative family and the local Boltzmann weights satisfy the Yang-Baxter equation [3].

There is an important function of Boltzmann weights of the model which is usually denoted by Δ (see [3], [10] and Section 3). The 6-vertex model with periodic boundary conditions has three phases in the thermodynamic limit, depending on the value of Δ . One is the totally ordered (frozen) phase, with $\Delta > 1$, the second is the disordered (critical) phase, with $|\Delta| < 1$, and the third is the partially ordered (antiferromagnetic) phase with $\Delta < -1$. The 6-vertex model can be used to describe electric or magnetic properties of crystals. Here we assume it is a model for magnetic properties. In [10] and many other papers it is regarded as a model for electric properties, so there are minor differences in terminology.

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Math. classification: 82-08, 88B20, 82B23.

The 6-vertex model with domain wall boundary conditions on a square $N \times N$ grid was perhaps first considered in [8] in the process of computation of norms of Bethe vectors. The partition function of this system can be written as the determinant of a certain $N \times N$ matrix [5]. Its asymptotics in the thermodynamic limit $N \rightarrow \infty$ were analyzed in [7]. It is related to matrix models, which was pointed out and exploited in [19]. But still, relatively little is known about this model.

The 6-vertex model with $\Delta = \frac{1}{2}$ is also known as the ice-model. This model with domain wall (DW) boundary conditions is closely related to the enumeration of alternating sign matrices [9]. It also has other interesting combinatorial features (see for example [17], [20]). When $\Delta = 0$ the 6-vertex model is equivalent to the problem of counting of weighted tilings of the Aztec diamond (see for example [7], [6] and references therein).

The spatial coexistence theory of different phases and the interfaces separating phases is an important part of statistical mechanics. Growth of crystals is one of the well known phenomena of this type. Limit shape effect in statistics of Young diagrams [18] and plane partitions [12], [13] are other closely related subjects.

In dimer models related to enumeration of plane partitions and domino tilings, the interface between the disordered and totally ordered phases is also known as an *arctic circle* phenomenon [1]. In these models the limit shapes or interfaces (curves separating phases), under broad conditions, are real algebraic curves [11]. Since at $\Delta = 0$ the 6-vertex model is equivalent to a dimer model these results imply that such a phenomenon exists in the 6-vertex model for $\Delta = 0$. The natural question is whether the spatial coexistence of phases happens only at the free fermionic point or if it occurs for all values of Δ . Numerical evidence suggesting the existence of a limit shape in the 6-vertex model with domain wall boundary conditions for all weights was obtained in [16].

Here we report results of numerical study of the 6-vertex model with DW boundary conditions in all phases of the model. Our method is different from [16]. To generate a random configuration in the 6-vertex model we construct the Markov process which is equivalent to a random weighted walk on the graph where the vertices are states of the model and edges are local moves which transform states into other states. This process satisfies the detailed balance condition and therefore converges to the Gibbs state of the 6-vertex model. Our process is also known as a Monte-Carlo process with local updates and as a heat-bath algorithm.

In statistical mechanics such processes are known as Kawasaki, or Glauber dynamics.

Since our goal was to collect “visual” evidence of the formation of the limit shape and qualitative information about it, we used a rather crude way to estimate the running time of Markov process. Specifically, we started computation simultaneously from the high and from the low height functions and we ran the simulation until a random state in the first process became visually indistinguishable from a random state in the second process. Clearly this would not be enough for any quantitative computations where a numerical error estimate is desired. We plan to address this in the future using the perfect sampling algorithm known as the “coupling from the past”, see [14].

Our results confirm the conclusion from [4] and [16] that there is a coexistence of ordered and disordered phases in the 6-vertex model. They also clearly indicate that for $\Delta < -1$ there is a coexistence of all three phases. The outer layer is an ordered phase. It is followed by a ring of the disordered phase vertices. Finally, there is an inner droplet of the antiferromagnetic phase. This phenomenon was first conjectured in [16] using a different numerical method. The shape of the inner droplet has four cusps and is reminiscent of one of the limit shapes for dimers on a square-octagon grid (see [11]) equivalent to the diablo tiling.

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1. Weights and local moves.

1.1. States.

States of the 6-vertex model on a square lattice are configurations of arrows assigned to each edge. The 6-vertex rule is that the total number of arrows coming into any vertex should be equal to the total number of arrows going out of this vertex. Each configuration of arrows can be equivalently regarded as a configuration of empty edges (arrows oriented South-North and East-West) and occupied edges, or thick edges (arrows pointing in the opposite directions). It is clear that thick edges will form paths. Possible configurations of paths around a vertex are shown on Fig. 1.1.

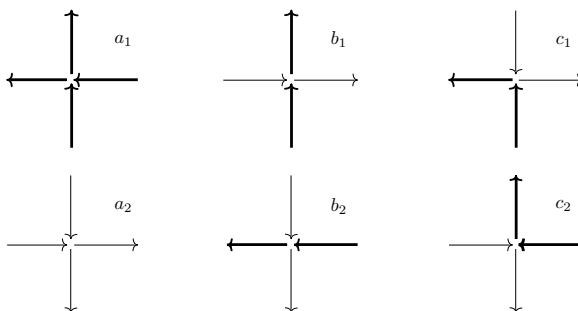


Figure 1. The six vertices and their weights

We will use $a_1, a_2, b_1, b_2, c_1,$ and c_2 as names of the vertices. We denote by the same letters Boltzmann weights assign to these vertices.

Domain wall boundary conditions are shown on Fig. 2 and 3.

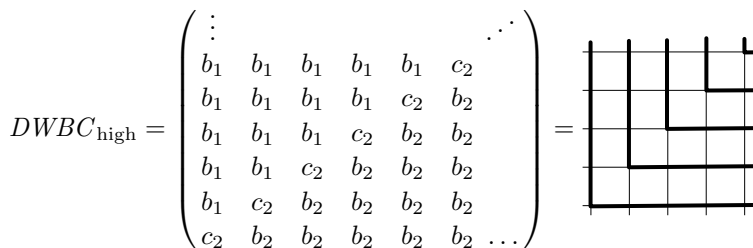


Figure 2. Domain wall boundary condition high (DWBC_H)

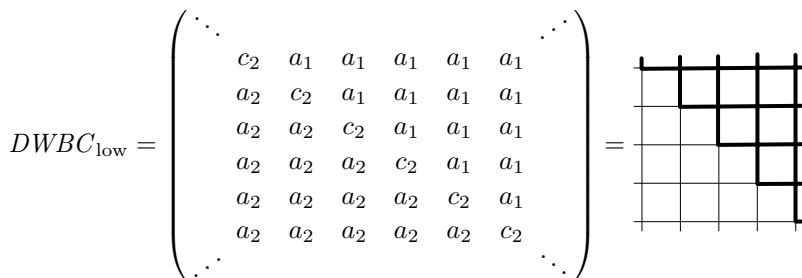


Figure 3. Domain wall boundary condition low (DWBC_L)

For domain wall boundary conditions every path in a 6-vertex configuration will have one end at the North boundary of the square and the other end at the East boundary of the square. These paths can be regarded as level curves of a height function. The lowest height function is shown on Fig. 3 and the highest height function is shown on Fig. 2.

1.2. Weights.

The weight of a state is the product of weights of vertices and the weight of a vertex is determined by rules from Fig. 1. The partition function is the sum of weights of all configurations:

$$Z_{6v} = \sum_{\text{states}} \prod_{\text{vertices}} w(\text{vertex, state})$$

where $w(\text{vertex, state})$ is the weight of the vertex (see Fig. 1).

The ratio

$$\frac{1}{Z_{6v}} \prod_{\text{vertices}} w(\text{vertex, state})$$

is the probability of the state. This is the Gibbs measure of the 6-vertex model.

1.3. Local moves and the graph of states.

Now let us describe local moves in the space of states. Such a move changes the configuration of arrows at the minimal number of edges near a given vertex and it acts transitively, i.e. any given state of the model can be transformed to any other given state of the model by a sequence of such moves.

Such moves are most transparent in terms of height functions. There are two types of local moves:

- The path from Fig. 4 we can move up, i.e. to the path from Fig. 5. We will call this move flip up.
- The path from Fig. 5 can be moved down, i.e. to the path from Fig. 4. We will say that this is the flip down.

$$S_a = \begin{pmatrix} b_1 & a_2 \\ c_2 & b_2 \end{pmatrix} = \begin{array}{|c|c|} \hline \text{---} & \text{---} \\ \hline \text{---} & \text{---} \\ \hline \end{array}$$

Figure 4. A local configuration that may be flipped up

$$S_b = \begin{pmatrix} c_2 & c_1 \\ a_2 & c_2 \end{pmatrix} = \begin{array}{|c|c|} \hline \text{---} & \text{---} \\ \hline \text{---} & \text{---} \\ \hline \end{array}$$

Figure 5. The local configuration after an up flip has occurred

Such moves with all possible surrounding configurations we will call flips up and down.

For each flippable vertex we introduce effective weight as follows:

- For a vertex flippable up the effective weight is the product of weights of all vertices that can be affected by the flip, i.e. the vertex itself, and the neighboring vertices to the North, the East, and the North-East of it.

- Similarly for a vertex flippable down the effective weight of it is the product of weights of the vertex itself, and of next neighboring vertices to the South, West, and South-West of it.

The effective weight is always the product of four factors. The effective weight of vertex v in the configuration S we denote by $W_v(S)$.

2. The Markov process.

2.1. General strategy.

Consider the abstract graph with vertices being states of the model and with edges being local moves. This graph is clearly connected. Our goal is to construct a random walk on this graph converging to the probabilistic measure on vertices of this graph which is the Gibbs measure of the 6-vertex model with DW boundary conditions.

Let us recall some basic facts. Let Γ be a finite connected graph and $q : V(\Gamma) \rightarrow \mathbb{R}_+$ be a probabilistic measure on the set of vertices of Γ . Let $M = \{p(a \rightarrow b)\}_{a,b \in V(\Gamma)}$ be the matrix of the Markov process describing a random walk on Γ . A traveler moves from a to b with the probability $p(a \rightarrow b)$.

The matrix M must satisfy the total probability condition

$$\sum_b p(a \rightarrow b) = 1.$$

If in addition it satisfies the detailed balance condition

$$q(a) p(a \rightarrow b) = q(b) p(b \rightarrow a)$$

then it is known that the Markov process converges to q . For details about Markov sampling and estimating convergence times, see [15].

Now our goal is to construct such a random walk converging to the Gibbs state of the 6-vertex model. At some point the rate of convergence of this Markov process becomes an important issue.

2.2. The Markov process for the 6-vertex model.

We want to construct a Markov process which chooses a vertex at random, then with the probability which we will describe below it will either flip the configuration up at this vertex, or will flip it down, or will do nothing. The probability of passing from the state S_a to the state S_b in this process can be written as follows:

$$\begin{aligned}
 (1) \quad P(S_a \Rightarrow S_b) &= \frac{1}{\# \text{ vertices}} \sum_v P_v(S_a \Rightarrow S_b) \\
 &= \frac{1}{\# \text{ vertices}} \left(\sum_{(v) \text{ non-flip}} \delta(S_a, S_b) + \sum_{(v) \text{ flip-up only}} P_v(S_a \Rightarrow S_b) \right. \\
 &\quad \left. + \sum_{(v) \text{ flip-down only}} P_v(S_a \Rightarrow S_b) + \sum_{(v) \text{ bi-flip}} P_v(S_a \Rightarrow S_b) \right) \\
 &= \frac{1}{\# \text{ vertices}} \left((\# \text{ non-flippable in } S_a) \delta_{S_a, S_b} \right. \\
 &\quad \left. + \sum_{(v) \text{ flip-up only}} P_v(S_a \Rightarrow S_b) + \sum_{(v) \text{ flip-down only}} P_v(S_a \Rightarrow S_b) \right. \\
 &\quad \left. + \sum_{(v) \text{ bi-flip}} P_v(S_a \Rightarrow S_b) \right) \\
 &= \frac{\# \text{ non-flippable}}{\# \text{ vertices}} \delta_{S_a, S_b} \\
 &\quad + \frac{\# \text{ flippable}}{\# \text{ vertices}} \left(\frac{1}{\# \text{ flippable}} \sum_{(v) \text{ flip-up only}} P_v(S_a \Rightarrow S_b) \right. \\
 &\quad \left. + \frac{1}{\# \text{ flippable}} \sum_{(v) \text{ flip-down only}} P_v(S_a \Rightarrow S_b) \right. \\
 &\quad \left. + \frac{1}{\# \text{ flippable}} \sum_{(v) \text{ bi-flip}} P_v(S_a \Rightarrow S_b) \right).
 \end{aligned}$$

Here # flippable is the number of flippable vertices and # vertices is the total number of vertices.

Algorithmically, this means that we do the following:

1) With probability

$$P = \frac{\# \text{ non-flippable}}{\# \text{ vertices}},$$

do nothing (that is, restart the loop).

2) With probability

$$P = \frac{\# \text{ flip-up-only} + \# \text{ flip-down-only} + \# \text{ bi-flip}}{\# \text{ vertices}} = \frac{\# \text{ flippable}}{\# \text{ vertices}},$$

continue to the next part.

If the algorithm continues, select a flippable vertex with the probability

$$(5) \quad P(\text{selection}) = \frac{1}{\# \text{ flippables}}$$

At this selected vertex the configuration can be either flippable only up, or only down, or in both directions. Depending on this proceed according to the following rules:

Three possible conditions now exist:

1) The vertex is flippable down only. Two options:

- Flip vertex down with probability $P_v(S_a \Rightarrow S_b) = \rho W_v(S_b)$,
- Stay with probability $P_v(\text{stay}) = 1 - \rho W_v(S_b)$.

2) The vertex is flippable up only. Two options:

- Flip vertex up with probability $P_v(S_a \Rightarrow S_b) = \rho W_v(S_b)$,
- Stay with probability $P_v(\text{stay}) = 1 - \rho W_v(S_b)$.

3) The vertex is flippable up and down. Three options:

- Flip vertex down with probability $P_v(S_a \Rightarrow S_b) = \rho W_v(S_b)$,
- Flip vertex up with probability $P_v(S_a \Rightarrow S_{b'}) = \rho W_v(S_{b'})$,
- Stay with probability $P_v(\text{stay}) = 1 - \rho W_v(S_b) - \rho W_v(S_{b'})$.

Here $W_v(S_{b'})$ $W_v(S_b)$ are the effective weights of the vertex v in the states obtained by flipping up or down at this vertex from the state S_a . Effective weights were described in Section 1.3.

The parameter ρ is chosen such that all probabilities of transitions should be positive. In other words it should satisfy all conditions $\rho < 1/W_v(S')$ where v is a vertex flippable in the state S either up or down, but not biflippable and S' is the configuration after the flip. At every biflippable vertex in the state S we should have $\rho < 1/(W_v(S') + W(S''))$ where S' is the result of the flipping S up at v and S'' is the result of the flip down.

This process satisfies the detailed balance condition, and the total probability condition. Since the graph of states with edges being local

moves is connected, this process converges to the Gibbs state of the 6-vertex model. The process also depends on the choice of ρ . It slows down when ρ is small.

3. Random states in the 6-vertex model with DW boundary conditions.

3.1. Phases in the 6-vertex model.

One can write weights of the 6-vertex model as

$$(6) \quad a_1 = \exp\left(-\frac{E_1 - H_x - H_y}{T}\right), \quad a_2 = \exp\left(-\frac{E_1 + H_x + H_y}{T}\right),$$

$$(7) \quad b_1 = \exp\left(-\frac{E_2 + H_x - H_y}{T}\right), \quad b_2 = \exp\left(-\frac{E_2 - H_x + H_y}{T}\right),$$

$$(8) \quad c_1 = c_2 = \exp\left(-\frac{E_3}{T}\right).$$

Here E_1, E_2 , and E_3 are energies of the interaction of arrows (or energies associated with the local shape of level curves of the height function) and H_x, H_y are magnetic fields.

In this interpretation arrows can be regarded as spins interacting with the magnetic field such that the energy of a vertical arrow is $\pm H_x$ depending on whether the arrow is heading up or down. The energy of a horizontal arrow is $\pm H_y$ depending on whether it is oriented left or right. We assigned the energy of an arrow to the energies of adjacent vertices.

Notice that since the total number of c_1 - and c_2 -vertices satisfies the relation $n(c_1) - n(c_2) = N$ the partition function changes by an overall factor only when we change c_1/c_2 . The total numbers of a and b vertices satisfy similar relations: $n(a_1) = n(a_2)$ and $n(b_1) = n(b_2)$. Because of this for the square lattice with DW boundary conditions we can set $a_1 = a_2 = a$, $b_1 = b_2 = b$, and $c_1 = c_2 = c$ without losing generality.

3.1.2. — Let us recall the phase diagram of the 6-vertex model [10], [3] with periodic boundary conditions in the absence of magnetic fields. The important characteristic of the model is the parameter

$$\Delta = \frac{a^2 + b^2 - c^2}{2ab}$$

The phase diagram for the 6-vertex model with periodic boundary conditions in the absence of magnetic fields is shown on Fig. 6.

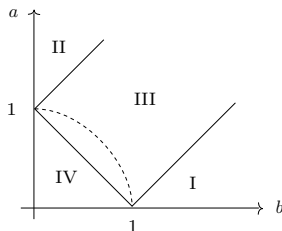


Figure 6. The phase diagram for the six-vertex model in terms of the weights of a and b , assuming $c = 1$.

There are four phases:

1) Phase I: $a > b + c$ ($\Delta > 1$). This is an ordered phase where there are two possibilities for the ground state. It either consists of a_1 -vertices or of a_2 -vertices. In either case any change in the ground state results in a state with the total number of b and c vertices comparable with the linear size N of the system. Thus, as $N \rightarrow \infty$ the energy of these two ground states is macroscopically separated from the energy of other states. In other words these are two frozen ground states.

2) Phase II: $b > a + c$ ($\Delta > 1$). This is an ordered phase with double degeneracy of the ground state. The first possibility is when all vertices are b_1 vertices, the second possibility is when all vertices are b_2 -vertices. As in case of phase I, this is a frozen phase.

3) Phase III: $a, b, c < \frac{1}{2}(a+b+c)$ ($|\Delta| < 1$). This is a disordered phase. Local correlation functions decay as a power of the distance in this phase. These are the values of a, b, c when $|\Delta| < 1$. In particular, the free fermionic curve $\Delta = 0$ lies entirely in this phase. It is shown by the dotted segment of the circle on Fig. 6.

4) Phase IV: $c > a + b$ ($\Delta < -1$). This is an ordered phase with so-called antiferromagnetic ordering (see Fig. 7). The ground state in this case consists of alternating c_1 and c_2 vertices. It is doubly degenerate due to the breaking of Z_2 -translational symmetry. In this case microscopic deviations from the ground state are possible. There is a finite correlation length in the system and local correlation functions decay exponentially.

For details about phase transitions, magnetization, and the antiferromagnetic phase, etc. see [10] and [3].

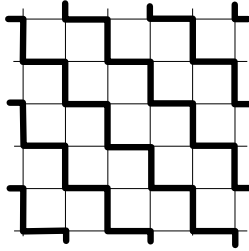


Figure 7. Antiferromagnetic phase – in this phase, zig-zag paths alternate with zig-zags formed by empty edges

3.2. The structure of a random state.

3.2.1. *Free fermionic point.* — This is the case when $\Delta = 0$. It is convenient to parameterize weights in this case as

$$a = \rho \cos u, \quad b = \rho \sin u, \quad c = \rho.$$

When $a = b = 1/\sqrt{2}$ this model is equivalent to the domino tiling of the Aztec diamond. The limit shape was computed analytically in [2] and is a circle.

The height functions of the average states for several values of the parameter u are shown on Fig. 8. For $\Delta = 0$, the limit shapes can be computed explicitly using methods of [11] and they are ellipses, which agrees with Fig. 8.

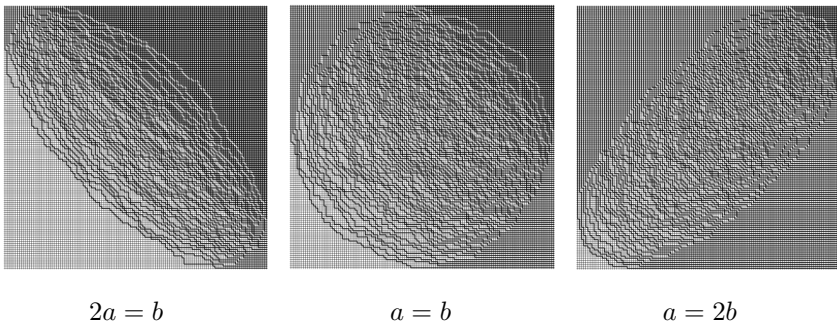


Figure 8. Free fermionic point with $\Delta = 0$

3.2.2. *Ordered phases.* — In Phase I the a -vertices dominate and the Gibbs state in this case is given by the lowest height function Fig. 3.

In Phase II the b vertices dominate and according to [10] we should expect that the average state will be the state with the domination of b -vertices. In other words the average state in this case is given by the highest height function Fig. 2.

3.2.3. *Disordered phase.* — In this case it is convenient to use the following parametrization of weights:

$$a = r \sin(\gamma - u), \quad b = r \sin u, \quad c = r \sin \gamma$$

with $0 < \gamma < \frac{1}{2}\pi$, $0 < u < \gamma$, and $r > 0$. In this parametrization $\Delta = \cos \gamma$, and

$$a = r \sin(u - \gamma), \quad b = r \sin u, \quad c = r \sin \gamma$$

where $0 < \gamma < \frac{1}{2}\pi$, $\gamma < u < \frac{1}{2}\pi$. In this case $\Delta = -\cos \gamma$.

Phase III contains the free fermionic curve $\Delta = 0$. Since this phase is critical, one may expect that the nature of the Gibbs states will be similar for all parameters a, b, c in this region. In particular, one would expect the existence of a limit shape as in the case $\Delta = 0$. The particular form of the limit shape may vary but the following common features should occur for all values of a, b, c in this region:

- The limit shape is a smooth curve having exactly one common point with each side of the square. At this point the limit shape is tangent to the side of the square.
- Inside of the boundary of the limit shape the height function is a smooth function and it has continuous first derivative at the boundary. The second derivative has a discontinuity in the normal direction to the boundary of the limit shape.
- Outside of the boundary of the limit shape the height function is linear.

Examples of Gibbs states in the disordered phase are shown on Fig. 9, 10, 11.

3.2.4. *The antiferromagnetic phase.* — This region $c > a + b$ is the one which is non-critical and which is also not ordered. In the periodic case the ground state has the domination of c -vertices as it is shown on Fig. 12.

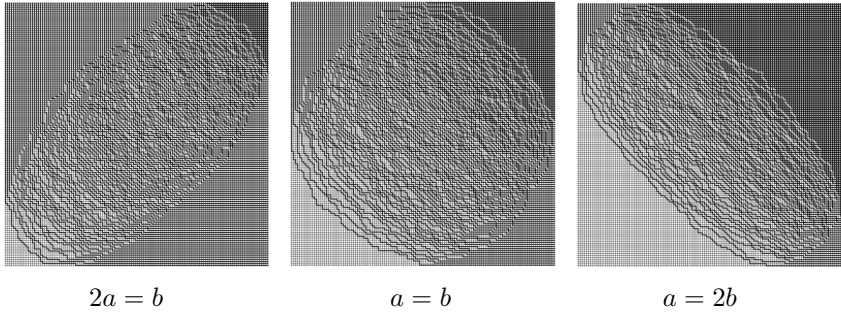


Figure 9. Disordered phase with $\gamma = \frac{1}{4}\pi$

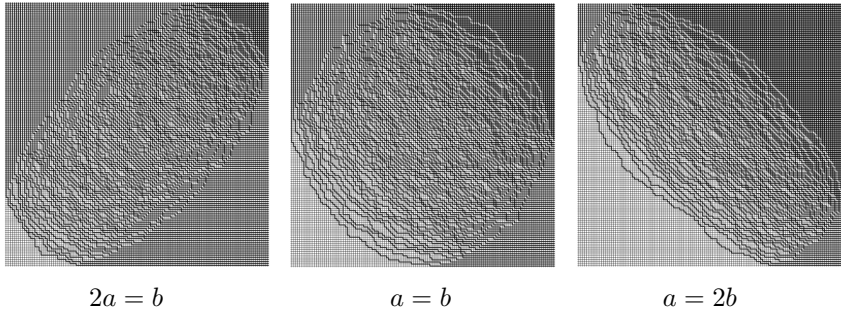


Figure 10. Disordered phase with $\gamma = \frac{1}{5}\pi$

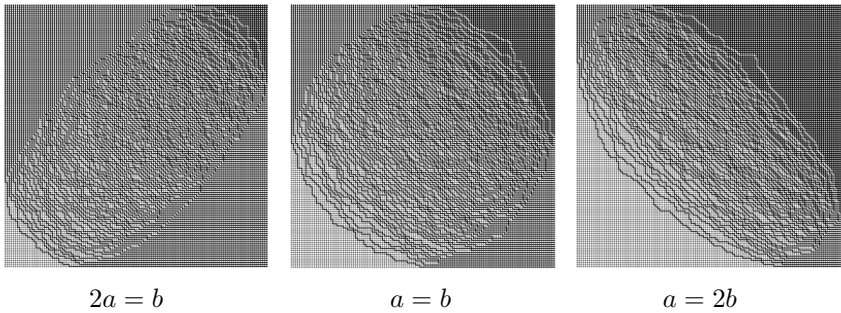


Figure 11. Disordered phase with $\gamma = \frac{1}{8}\pi$

It is convenient to use the parameterization

$$a = r \sinh(\eta - u), \quad b = r \sinh u, \quad c = r \sinh \eta$$

with $0 < u < \eta$. In this parametrization $\Delta = -\cosh \eta$.

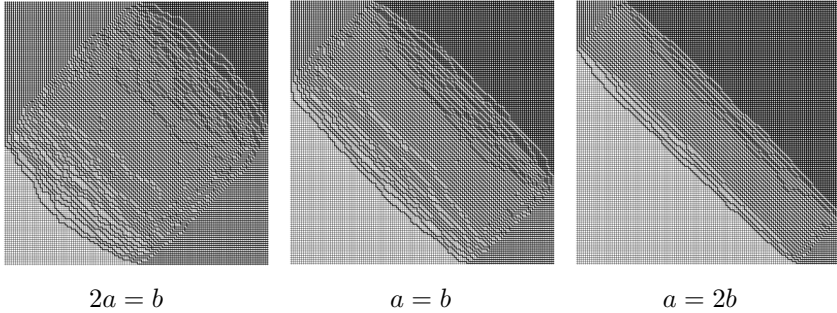


Figure 12. Antiferromagnetic phase with $\Delta = -3$

In the case of DW boundary conditions there is a competition between very rigid restrictions on the states near the boundary which allows only a and b vertices near the boundary and the tendency of the system to have as many c vertices as possible.

Numerical simulations show that these competing tendencies resolve in the separation of three phases. It is fairly convincing from the Fig. 12 that the following should take place:

- The system forms a macroscopical droplet of the antiferromagnetic phase with a boundary that does not touch the square. The height function in this domain is linear. The boundary of this domain has four cusps pointing towards sides of the square lattice. This phase is noncritical. Correlation functions in this region decay exponentially.

- Near the boundary the system is ordered. This ordered region is bordered by the disordered region where the height function is smooth. The disordered phase is critical. There is a finite magnetization, which means there are excitations with linear dispersions and therefore correlation functions decay according to a power law. The boundary between ordered and disordered phases is a smooth curve with the features similar to the $|\Delta| < 1$ case.

4. Conclusion.

We demonstrated that local Markov sampling for the 6-vertex model with domain wall boundary conditions indicates that the system develops a macroscopical droplet of c -vertices when $\Delta < -1$. Though the existence of the droplet can be seen from results of [16] its actual shape is very

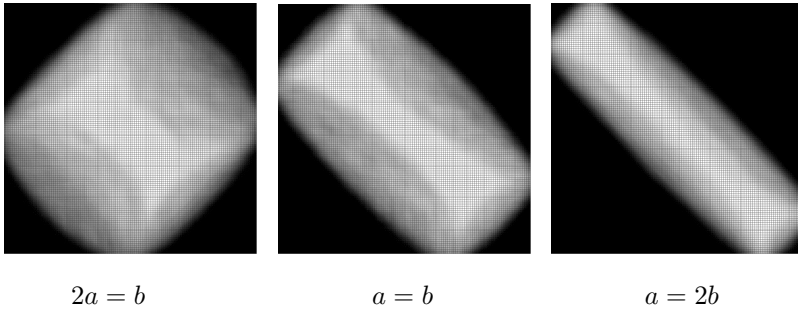


Figure 13. c -density plots of the antiferromagnetic phase with $\Delta = -3$

difficult to see there. For our computations it is not essential that the ground state of the 6-vertex model in this phase is doubly degenerate. This degeneracy corresponds to the translation by one step in the North-East direction on Fig. 12. However, this degeneracy is important and presents difficulties in the computation of correlation functions and other observable features. In [16] this problem was properly addressed and some interesting numerical results about correlation functions were obtained.

As it was mentioned in the introduction we did not estimate the running time of the Markov process but the data strongly suggest that it is polynomial in N .

It is interesting that the droplet of c -vertices is similar to the facets in dimer models. The shape of the droplet and of the surrounding critical phase is similar to the corresponding shapes in the dimer model on the square-octagon lattice (see [11]). Notice that singularities in the limit shape are cusps just as in the dimer models (see [13] and unpublished talks by Kenyon and Okounkov).

The local Markov sampling which we used here is equally effective for other boundary conditions in the 6-vertex model. Some of the results for more complicated boundary conditions for the uniformly distributed ($a = b = c = 1$) 6-vertex model (ice model) can be found in [4].

The questions of the speed of convergence and the results of sampling for other fixed boundary conditions for the 6-vertex model will be addressed in a separate publication.

A puzzling question is the role of integrability. The phenomenon of the formation of the limit shape, also known as the large deviation principle is a general phenomenon. The integrability most likely plays no role in it.

However, the specific features of the limit shape may be very special for integrable systems. It would be very interesting to understand this.

A. Functions and Implementations.

A.1. Main loop.

The following tasks must be completed by the *Main Loop* function:

- 1) Import the matrix from a text file.
- 2) Build flippables list.
- 2) Set weights.
- 3) Define

$$(9) \quad \rho = \frac{1}{\max\{\text{weight combinations for all flip types}\}}.$$

5) Loop the following actions, and after a certain defined number of successful flips, output a file with the current matrix (and status of the Markov Chain) in it:

- (a) Generate a random real, *rand*, between 0 and 1,
 - (i) continue to (b) if

$$\frac{\#\text{flip-up-only} + \#\text{flip-down-only} + \#\text{bi-flip}}{\#\text{vertices}} \geq \text{rand},$$

- (ii) otherwise, go to (a).
- (b) Select a random flippable position with probability

$$P(\text{selection}) = \frac{1}{\#\text{flip-up-only} + \#\text{flip-down-only} + \#\text{bi-flip}}$$

by calling the *Get Flippable Position* function.

- (c) Call *Get Weight* (which is now scaled by the value of ρ , to ensure that it always returns a value less than 1) to get the probability of an up flip and/or a downflip at the flippable location chosen.
- (d) Generate a random real, *rand*, between 0 and 1,

- (i) for up or down-only flips, iff $W(S_b) \geq \text{rand}$, execute the flip by calling the *Execute Flip* function, else restart main loop;
- (ii) for positions that can flip up and down, iff $W(S_b) \geq \text{rand}$, execute the flip corresponding to S_b , else iff $W(S_{b'}) \geq \text{rand}$, execute the flip corresponding the $S_{b'}$, else restart main loop. In practice, this means that once a vertex which can be flipped either way is chosen, simply divide up the probabilities of each flip occurring as discussed earlier.

A.2. Execute Flip.

1) If type is high:

- (a) Change the entry in the list of *Flippables* for the vertex chosen to make a high flip impossible.
- (b) Define the following positions:
 - (i) *One* = the original position = *Base*
 - (ii) *Two* = (+1, +0) = *Right*
 - (iii) *Three* = (+1, +1) = *UpRight*
 - (iv) *Four* = (+0, +1) = *Up*
 - (v) *Left* = (-1, +0)
 - (vi) *Down* = (+0, -1)
 - (vii) *UpLeft* = (-1, +1)
 - (viii) *UpRight* = (+1, +1)
 - (ix) *DownLeft* = (-1, -1)
 - (x) *DownRight* = (+1, -1)
- (c) Replace four parts:
 - (i) Set Contents of *Position One*

$$= \text{FlipToOne}(\text{Position One}, \text{High})$$
 - (ii) Set Contents of *Position Two*

$$= \text{FlipToTwo}(\text{Position Two}, \text{High})$$
 - (iii) Set Contents of *Position Three*

$$= \text{FlipToThree}(\text{Position Three}, \text{High})$$
 - (iv) Set Contents of *Position Four*

$$= \text{FlipToFour}(\text{Position Four}, \text{High})$$

- (d) If *Up*, *Down*, *Right*, or *Left* Positions become flippable (call *Get Is Flippable* on each to check), add them to the *Flippables* list.
- (e) Call *Fix Low End*.
- 2) If type is low:
- (a) Change the entry in the list of *Flippables* for the entry chosen to make a low flip impossible.
- (b) Define the following positions:
- (i) $One = (-1, -1) = \textit{DownLeft}$
 - (ii) $Two = (+0, -1) = \textit{Down}$
 - (iii) $Three = \text{the original position} = \textit{Base}$
 - (iv) $Four = (-1, +0) = \textit{Left}$
 - (v) $Right = (+1, +0)$
 - (vi) $Up = (+0, +1)$
 - (vii) $UpLeft = (-1, +1)$
 - (viii) $UpRight = (+1, +1)$
 - (ix) $DownLeft = (-1, -1)$
 - (x) $DownRight = (+1, -1)$
- (c) Replace four parts:
- (i) Set Contents of Position *One*
 $= \textit{FlipToOne}(\textit{PositionOne}, \textit{Low})$
 - (ii) Set Contents of Position *Two*
 $= \textit{FlipToTwo}(\textit{PositionTwo}, \textit{Low})$
 - (iii) Set Contents of Position *Three*
 $= \textit{FlipToThree}(\textit{PositionThree}, \textit{Low})$
 - (iiii) Set Contents of Position *Four*
 $= \textit{FlipToFour}(\textit{PositionFour}, \textit{Low})$
- (d) If *Up*, *Down*, *Right*, or *Left* Positions become flippable (call *Get Is Flippable* on each to check), add them to the *Flippables* list.
- (e) Call *Fix High End*.

A.2.1. *Fix High End*

- 1) Define the following positions:
- (a) $\textit{HighCreateDownLeft} = (-1, -1)$
 - (b) $\textit{HighDeleteDown} = (+0, -1)$

- (c) $HighDeleteDownDownLeft = (-1, -2)$
- (d) $HighDeleteDownRightLeft = (-2, -1)$
- (e) $HighDeleteLeft = (-1, +0)$

2) If $HighCreateDownLeft$ is flippable, add it to the *High Flippables* list.

3) Delete four potential flippables on the *High End*.

4) If any of $HighDeleteDown$, $HighDeleteDownDownLeft$, $HighDeleteDownLeftLeft$, or $HighDeleteLeft$ exists in the *High Flippables* list, remove them from the list.

A.2.2. *Fix Low End*

1) Define the following positions:

- (a) $LowCreateUpRight = (+1, +1)$
- (b) $LowDeleteUp = (+0, +1)$
- (c) $LowDeleteUpUpRight = (+1, +2)$
- (d) $LowDeleteUpRightRight = (+2, +1)$
- (e) $LowDeleteRight = (+1, +0)$

2) If $LowCreateUpRight$ is flippable, add it to the *Low Flippables* list.

3) Delete four potential flippables on the *Low End*.

4) If any of $LowDeleteUp$, $LowDeleteUpUpRight$, $LowDeleteUpRightRight$, or $LowDeleteRight$ exists in the *Low Flippables* list, remove them from the list.

A.3. Get Weight.

1) Get contents of four surrounding positions if the flip occurred.

2) Multiply weights together corresponding to the contents of the four positions.

3) Multiply (new weight configuration product) by ρ .

A.4. Flip To.

FlipTo functions take a position and a type and return what the vertex at the given position would be after the flip of the type specified.

1) $FlipToOne(Position, Type)$

- (a) If type is high: If vertex was a_1 , it will be c_1 ; if it was c_2 , it will be a_2

- (b) If type is low: If vertex was c_1 , it will be a_1 ; if it was a_2 , it will be c_2
- 2) *FlipToTwo*
 - (a) If type is high: If vertex was b_2 , it will be c_2 ; if it was c_1 , it will be b_1
 - (b) If type is low: If vertex was c_2 , it will be b_2 ; if it was b_1 , it will be c_1
- 3) *FlipToThree*
 - (a) If type is high: If vertex was a_2 , it will be c_1 ; if it was c_2 , it will be a_1
 - (b) If type is low: If vertex was c_1 , it will be a_2 ; if it was a_1 , it will be c_2
- 4) *FlipToFour*
 - (a) If type is high: If vertex was b_1 , it will be c_2 ; if it was c_1 , it will be b_2
 - (b) If type is low: If vertex was c_2 , it will be b_1 ; if it was b_2 , it will be c_1

A.5. Get Flip Position.

1) Generate a random integer between 1 and the total number of flippable positions; that is, the number of up-flip only plus the number of down-flip only plus the number of bi-flips.

2) Choose the corresponding element in the *Flippable Positions* list to the random number chosen.

A.6. Get Is Flippable.

Get Is Flippable should check the status of a position to determine if it is flippable.

1) High flippables must be a_1 or c_2 vertices and must have empty upper right corners (upper right corner must be a_2 or c_2). High flippable positions must have an x axis coordinate that is less than or equal to the width of the matrix 1 (where 0, 0 is the origin) and a y axis coordinate that is less than or equal to the height of the matrix 1.

2) Low flippables must be a_1 or c_1 vertices and must have empty lower left corners (lower left corner must be a_2 or c_1). Low flippable positions must have an x axis coordinate that is no less than 1 (where 0, 0 is the origin), and a y axis coordinate that is no less than 1.

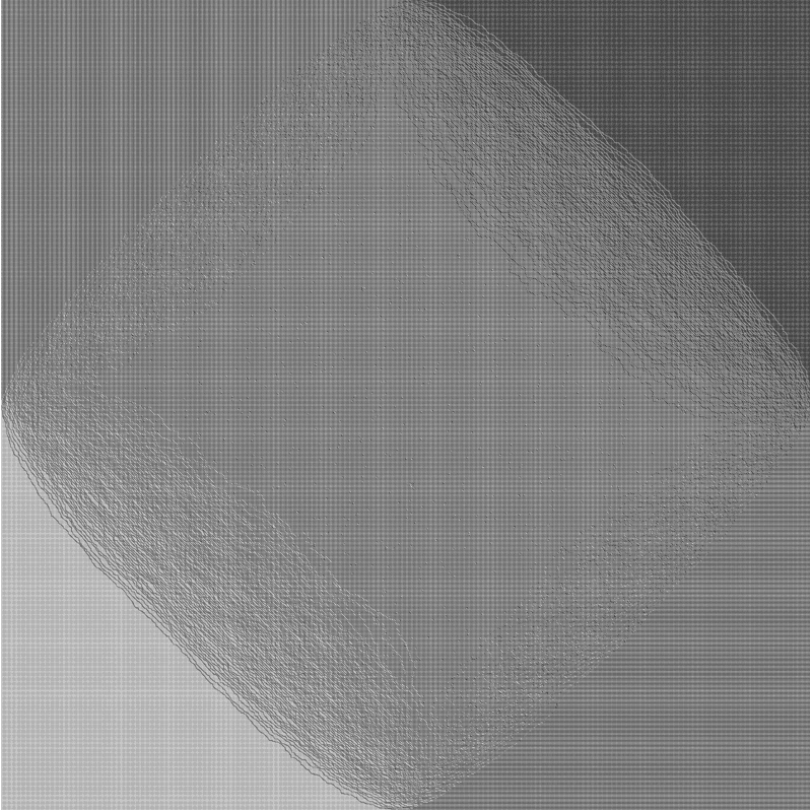
B. Images of the $N = 1000$ matrix.

Figure 14. $N = 1000$ plot for the antiferromagnetic phase with $\Delta = -3$ and $2a = b$

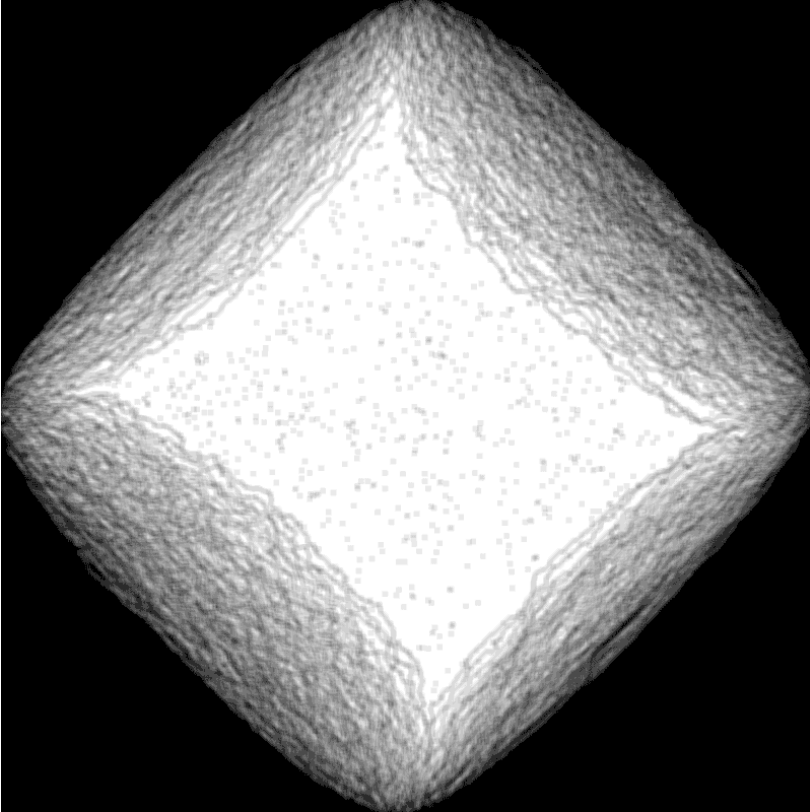


Figure 15. $N = 1000$ c -vertex density plot for the antiferromagnetic phase with $\Delta = -3$ and $2a = b$

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