Influence of boundary conditions on bulk properties of six-vertex model

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Received 29 July 2015
Accepted for publication 14 September 2015
Published 20 October 2015

Abstract
We study the influence of boundary conditions on the entropy of the six-vertex model. We consider the case of fixed boundary conditions in order to argue that the entropy of the six-vertex model vary continuously from its value for ferroelectric to periodic boundary conditions. This is done by merging the ferroelectric boundary and the Néel boundary.

Keywords: six-vertex model, boundary conditions, entropy

(Some figures may appear in colour only in the online journal)

1. Introduction

The six-vertex model is one of the simplest and most important exactly solvable models in statistical mechanics and it has been extensively studied over the years [1, 2]. Despite its simplicity, the six-vertex model provides a good description of the ice and spin-ice systems [3, 4].

This model was firstly solved with periodic boundary conditions [5]. Afterwards, the equivalence of the six-vertex model with free and periodic boundary conditions was shown in [6]. Additionally, it was noted that the free-energy of the six-vertex model cannot be independent of boundary conditions [6].

The dependence of the six-vertex on boundary conditions has also been investigated. The case of special free boundaries [7], anti-periodic boundaries [8] gave the same answers as the periodic boundary conditions. Later on, the six-vertex model with domain wall (DW)
boundary was considered. It was proved that it produces different bulk properties in the thermodynamic limit \cite{9-11}, e.g. the entropy at the ice-point is \( S_{DW} = \frac{1}{2} \ln \left( \frac{2}{3} \right) \). Recently the case of DW and reflecting end boundary condition was considered. It was also shown that the bulk properties differ from the periodic case \cite{12}.

This scenario fostered a systematic investigation of the influence of boundary conditions on six-vertex model bulk properties. It was recently shown that the bulk properties depend on the boundary conditions only when one has fixed boundary \cite{13}. In other words, this implies that periodic, anti-periodic and any mixture of periodic and anti-periodic along vertical and/or horizontal direction in the rectangular lattice produce the same bulk properties.

Nevertheless, it was also introduced in \cite{13} additional examples of fixed boundary conditions which produce different values for the entropy per lattice site. In particular, it was argued in that the entropy of the six-vertex model at the ice-point varies continuously from its value for ferroelectric boundary condition \( S_{FE} = 0 \) to its values with periodic boundary \( S_{PBC} = \frac{1}{2} \ln \left( \frac{3}{2} \right) \). However in \cite{13} it was only discussed the interval \( S_{FE} < S < S_{DW} \). The purpose of this paper is to review the previous results and extend them for the whole interval \( S_{FE} < S < S_{PBC} \) by means of the direct computation of the entropy per lattice site for finite lattices. This is done by merging the ferroelectric and Néel boundary conditions at certain fractions.

The outline of the article is as follows. In section 2, we describe the six-vertex model and its boundary conditions. In section 3, we discuss several instances of fixed boundary conditions. In section 4, we introduce another fixed boundary condition by merging the ferroelectric and Néel boundary and provide some data showing that indeed the entropy is within the interval \( S_{FE} < S < S_{PBC} \). Our conclusions are given in section 6.

2. The six-vertex model

In this section, we introduce the six-vertex model and its partition function with various fixed boundary conditions.

In general, the partition function of a vertex model can be written as a sum of all configurations \( \epsilon \),

\[
Z = \sum_{\epsilon} \prod_{i=1}^{N} \prod_{j=1}^{L} \omega^{\epsilon(i,j)},
\]

which is a complicated combinatorial problem. The weight \( \omega^{\epsilon(i,j)} \) can assume the values \( a(\lambda) \), \( b(\lambda) \) and \( c(\lambda) \), which are associated to the different vertex configurations of the six-vertex model (see figure 1) \cite{1}.

These Boltzmann weights are the matrix elements of the so called \( R \)-matrix \cite{1,2}, which is the key ingredient for the integrability and fulfill the famous Yang–Baxter equation \cite{1}.
3. Fixed boundary conditions

In this section we discuss some examples of boundary conditions which influence the bulk properties of the six-vertex model. We conveniently consider the case of square lattices $L = N$ throughout this work.

3.1. Ferroelectric boundary condition

The case of ferroelectric (FE) boundary condition is trivial in the sense that one has only one allowed physical state for any finite system size (see figure 2). Therefore, the partition
function is trivial for any values of the physical parameters. This is a direct consequence of the ice rule [6] and it implies that the entropy is zero ($S_{\text{FE}} = 0$).

3.2. DW boundary condition

The first non-trivial case was introduced long ago in the context of scalar products of the Bethe states. The partition function with the DW boundary condition (see figure 3) [14],

$$Z_N^{\text{DW}} (\{ \lambda \}, \{ \mu \}) = \langle \downarrow | B(\lambda_1) \cdots B(\lambda_N) B(\lambda_1) | \uparrow \rangle,$$

(2)

can be written as a determinant [15, 16]. This is a fundamental property which allowed for the computation of the bulk properties in the thermodynamic limit of the six-vertex model with DWBC [9–11]. This also established a relation with combinatorics, which is connected with the problem of counting the number of alternating sign matrices [17, 18].

3.3. Néel boundary condition

Recently, it was introduced the case of called Néel boundary condition or anti-ferroelectric boundary [13]. This is the case where we have the alternation of the arrows along the boundaries, see figure 4.

In contrast with the case of ferroelectric boundary condition which allows for only one possible state, the Néel boundary is the one which allows for the largest number of configurations. As a consequence of the arrows alternation in the boundary, it allows the largest number of arrow reversals along the boundary and this propagates to the bulk. It was shown in [13] that $S_{\text{NE}} = S_{\text{PBC}}$ at ice-point ($a = b = c = 1$) in the thermodynamic limit.

However, it was not possible to derive a product formula for the number of states involving factorials for the Néel boundary. The only estimates was obtained from the data for finite system size up to $N = 20$, which indicates that the entropy behaves as $S_{\text{NE}} = S_{\text{PBC}} \left( 1 - \frac{2}{N} \right)$, where $\gamma \sim 2$ [13]. Interesting enough, the Néel boundary conditions also appears in the context of generalized alternating sign matrices [19].
3.4. Merge of DW and FE boundary condition

We can generate additional boundaries by merging the previous cases. This results in different values for the bulk properties. By merging the DW and ferroelectric boundary, we have a smaller number of physical states and therefore the entropy is smaller than the DW boundary.

We build that by choosing an integer number \( n \) between 0 and \( N \). Starting from the upper-left corner, we fill the first \( n \) boundary row and column edges with arrows in the same way we would fill the DW boundary, see figure 5. The opposite edges of these are also filled with the respective arrows of the opposite edges of the DW boundary condition. So far, we have used the arrows configuration of a DW boundary with lattice size \( n \) to fill our boundary of lattice size \( N \). The remaining arrows are filled in the same way, but using boundary arrows of the ferroelectric boundary.

This implies that we have partially frozen the arrow configurations of the lattice in a similar way as the ferroelectric boundary. The difference lies in the \( n \times n \) sublattice at the upper-left corner. This implies we are left with a DW partition function of size \( n \), which means

\[
Z_{\text{DW-FE}}^n = \left[ \prod_{i=1}^{N} \prod_{j=n+1}^{N} b(\lambda_i - \mu_j) \right] \left[ \prod_{i=n+1}^{N} \prod_{j=1}^{n} a(\lambda_i - \mu_j) \right] \times Z_{\text{DW}}^n.
\]

Therefore, we see that the entropy at infinity temperature (ice-point) is given by

\[
S_{\text{DW-FE}} = \lim_{N \to \infty} \left( \frac{n}{N} \right)^2 S_{\text{DW}}.
\]

For a suitably chosen sequence \( n(N) \), one can obtain any value of entropy \( S \) in the interval \( S_{\text{FE}} \leq S \leq S_{\text{DW}} \) [13]. Therefore, the merge of DW and ferroelectric boundary condition implies that the entropy vary from its values for the ferroelectric case to the DW boundary case. However this leaves the interval \( S_{\text{DW}} \leq S \leq S_{\text{PBC}} \) as an open problem.

**Figure 5.** The partition function \( Z_{\text{DW-FE}}^n \) for \( N = 5 \) of the six-vertex model whose boundary are a mixture of the domain wall and ferroelectric boundary (DW–FE).
We consider the merge of the Néel and ferroelectric boundary in order to show that the entropy of the six-vertex model can vary in the whole interval $S_{\text{FE}} \leq S \leq S_{\text{PBC}}$. We have chosen the upper-left corner to be of Néel type and the lower-right corner to be of ferroelectric type, figure 6.

Taking into account the internal frozen degrees of freedom, one finds that the partition function takes the form of a L-shaped lattice rather than the usual rectangular one. This type of partition function have been investigated in the literature[20] with different boundary conditions.

By construction, we have that $S_{\text{NE-FE}} = S_{\text{FE}} = 0$ for $n = 0$ and $S_{\text{NE-FE}} = S_{\text{NE}} = S_{\text{PBC}}$ for $n = N$ which holds true in the thermodynamic limit. We argue that if $n$ changes from $n_0$ to $n_0 + 1$ there is a small variation in the entropy, as expected for large $N$ values. This is
supported in figure 7, where we show the entropy with fixed \( N = 20 \) and \( n \) ranging from 0 to \( N \).

With \( N \) as large as 20, we already can see the continuity taking place. The largest difference of consecutive entropies is less than 0.03. It reasonable to assume that

\[
S^{\text{NE-FE}}_{n+1} - S^{\text{NE-FE}}_n = O\left(\frac{1}{N}\right)
\]

To support this, we also show the entropy difference

\[
S^{\text{NE-FE}}_{n+1} - S^{\text{NE-FE}}_n \quad \text{with} \quad n = \left\lfloor \frac{N}{2} \right\rfloor
\]

and \( N \) ranging from 2 to 20, figure 8. As we can see, the entropy difference vanishes sufficiently fast.

5. Open problems

• Classify the boundaries conditions into classes, which produce the same entropy per lattice site in thermodynamic limit.
• Prove that the bulk free energy is constant inside of each class.
• Find new boundary conditions, for which the model is solvable analytically.
• Prove that for majority of boundary evaluation of bulk free energy is NP hard.
• Prove that for majority of boundary conditions the phase boundaries (in the space of Boltzmann weights) are the same as for periodic case.

6. Conclusion

In this paper we have studied the dependence of physical quantities, like entropy, of the six-vertex model on boundary conditions.

We argued that the entropy per lattice site changes continuously from zero to its value with periodic boundary condition in the thermodynamic limit.

There still remains open questions, e.g. the complete classification of the boundary conditions, the existence of further boundary conditions for which the model is solvable analytically and the existence of other vertex models whose physical quantities do depend on the boundary conditions.
Acknowledgments

TS Tavares and GAP Ribeiro thank the Galileo Galilei Institute and the organizers of the scientific program ‘Statistical Mechanics, Integrability and Combinatorics’ for hospitality and support during part of this work and the São Paulo Research Foundation (FAPESP) for financial support through the grants 2013/17338-4 and 2015/01643-8. VE Korepin was supported by NSF Grant DMS 1205422.

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