# Thermodynamic limit of the six-vertex model with reflecting end

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# Outline

- Problem
- Six-vertex model
- DWBC
- Reflecting
- determinant formula
- Homegeneous limit
- Special solution
- Entropy

# Problem

- In statistical physics people believe that in thermodynamic limit the bulk free energy and correlations should not depend on boundary conditions. This is often true, but there are counterexamples.
- One of the most proeminent one is the six-vertex model: PBC $\neq$ DWBC.
- We would like to compute the free-energy and entropy of the six-vertex model with boundaries different boundaries: reflecting end.
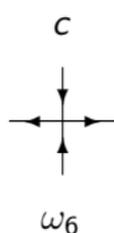
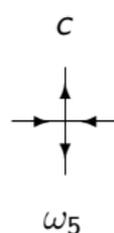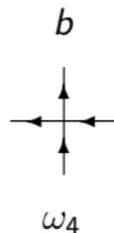# Water molecule x ice: six-vertex model

- Water molecule: O-H distance (0.95 $\mathring{A}$); angle between O-H: $104°$

- Ice: X-ray data (1930s) indicates that O form a hexagonal wurtzite structure (tetraedral): O-O distance (2.76 $\mathring{A}$)
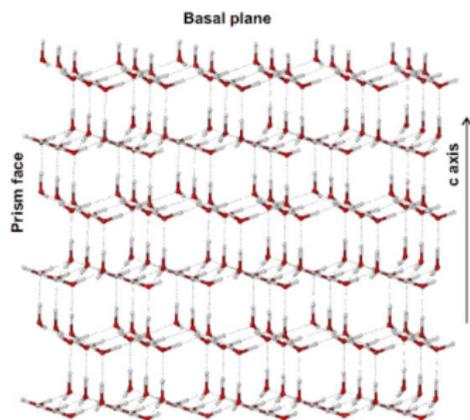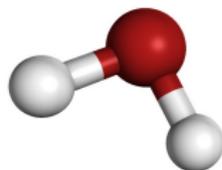
# Square-ice model: six-vertex model

$\Rightarrow$ Effective model: square ice-model.





| $a$ | $a$ | $b$ | $b$ | $c$ | $c$ |
|-----|-----|-----|-----|-----|-----|



| $\omega_1$ | $\omega_2$ | $\omega_3$ | $\omega_4$ | $\omega_5$ | $\omega_6$ |

$$\omega_i = e^{-\beta \varepsilon_i}$$

# Entropy

$$S = Nk \log W$$

$$
\begin{array}{cccc}
\text{H} - \text{O} & \text{H} - \text{O} - \text{H} & \text{O} - \text{H} & \text{O} - \text{H} \\
\quad | & \quad \text{H} & \quad | & \quad | \\
\quad \text{H} & & \quad \text{H} & \quad \text{H} \\
\text{H} - \text{O} - \text{H} & \text{O} & \text{H} - \text{O} - \text{H} & \text{O} - \text{H} \\
\quad \text{H} & \quad | & \quad \text{H} & \quad \text{H} \\
& \quad \text{H} & & \\
\text{H} - \text{O} & \text{H} - \text{O} & \text{H} - \text{O} & \text{H} - \text{O} - \text{H} \\
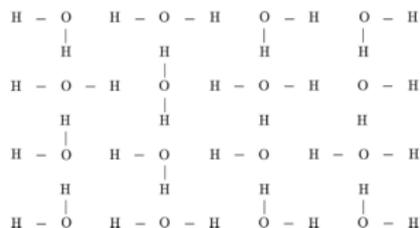\quad \text{H} & \quad | & \quad \text{H} & \quad \text{H} \\
\quad | & \quad \text{H} & \quad | & \quad | \\
\text{H} - \text{O} & \text{H} - \text{O} - \text{H} & \text{O} - \text{H} & \text{O} - \text{H}
\end{array}
$$
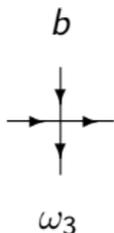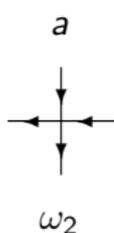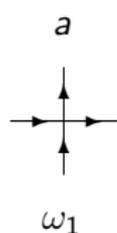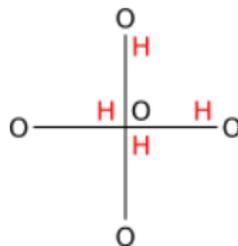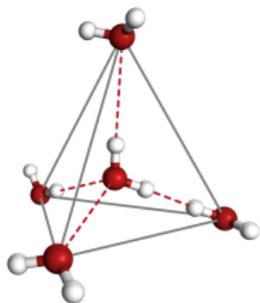
$\Rightarrow \varepsilon_1 = \varepsilon_2 = \cdots = \varepsilon_6 = 0$ (or $a = b = c = 1$).

- Pauling (1935) - estimated the entropy of the hexagonal phase of ice (ordinary ice): $W = 2^2 (6/16) = \frac{3}{2}$

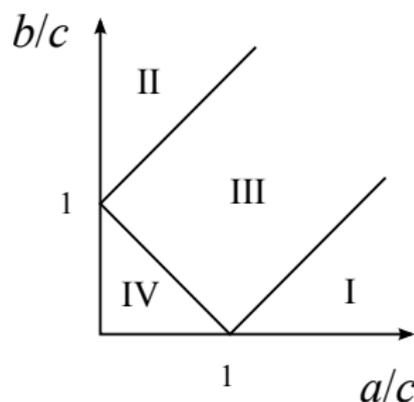- Lieb (1967) - computed exactly the entropy for the square-ice: $W = (\frac{4}{3})^{3/2} = 1.5396007\ldots$.

# Phases: six-vertex model

Control parameter is $\Delta = \dfrac{a^2 + b^2 - c^2}{2ab}$.

Free energy has different analytic forms when

- $\Delta > 1$ (ferroelectric).
- $-1 < \Delta < 1$ (disordered).
- $\Delta < -1$ (anti-ferroelectric).

# Phase diagram



- ▶ Phase I and Phase II (ferroelectric).
- ▶ Phase III (disordered).
- ▶ Phase IV (anti-ferroelectric).

This phase diagram describes the six-vertex model with PBC (Lieb 1967,Sutherland 1967, Baxter 1982) and with DWBC (V Korepin, P Zinn-Justin 2000, P Zinn-Justin 2000). Rigourous proofs are due P Bleher et al 2006,2009,2010...
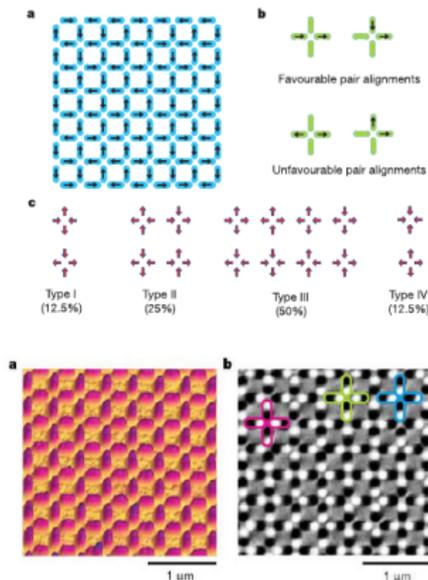
# Recent realization of vertex models

nature

LETTERS

## Artificial 'spin ice' in a geometrically frustrated lattice of nanoscale ferromagnetic islands

R. F. Wang[1], C. Nisoli[1], R. S. Freitas[1], J. Li[1], W. McConville[1], B. J. Cooley[1], M. S. Lund[1], N. Samarth[1], C. Leighton[2], V. H. Crespi[1] & P. Schiffer[1]

Figure 2 | AFM and MFM images of a frustrated lattice. a, An AFM image of a typical permalloy array with lattice spacing of 400 nm. b, An MFM image taken from the same array. Note the single-domain character of the islands, as indicated by the division of each island into black and white halves. The moment configuration of the MFM image is illustrated in Fig. 1a. The coloured outlines indicate examples of vertices of types I, II and III in pink, blue and green respectively.

PHYSICAL REVIEW LETTERS

## Effective Temperature in an Interacting Vertex System: Theory and Experiment on Artificial Spin Ice

Cristiano Nisoli,[1] Jie Li,[2] Xianglin Ke,[2] D. Garand,[2] Peter Schiffer,[2] and Vincent H. Crespi[2]
[1]Theoretical Division and Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA
[2]Department of Physics and Materials Research Institute, The Pennsylvania State University, University Park, Pennsylvania 16802, USA
(Received 16 December 2009; published 23 July 2010)
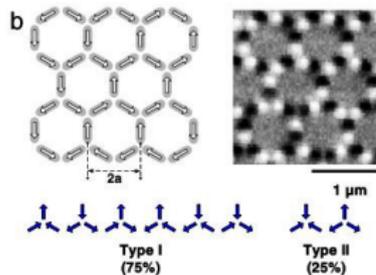
FIG. 1 (color online). Square and hexagonal artificial spin ice. (a) Schematics (top left) and MFM (top right) of the square arrays and the 16 vertices of the square artificial ice (bottom). (b) Schematics (top left) and MFM (top right) of the hexagonal arrays with 8 vertices of the hexagonal. White arrows show the vertex ground states, and the percentages indicate the vertex multiplicity.
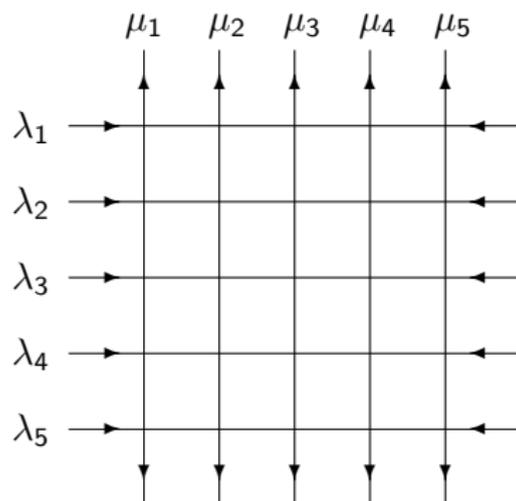
# DWBC

In the computation of scalar product os Bethe states,

$$|\psi\rangle_N = B(\lambda_N) \cdots B(\lambda_2) B(\lambda_1) |\Uparrow\rangle,$$

appears the (Korepin 1982)

$$Z_N^{DWBC}(\{\lambda\}, \{\mu\}) = \langle\Downarrow| B(\lambda_N) \cdots B(\lambda_2) B(\lambda_1) |\Uparrow\rangle.$$

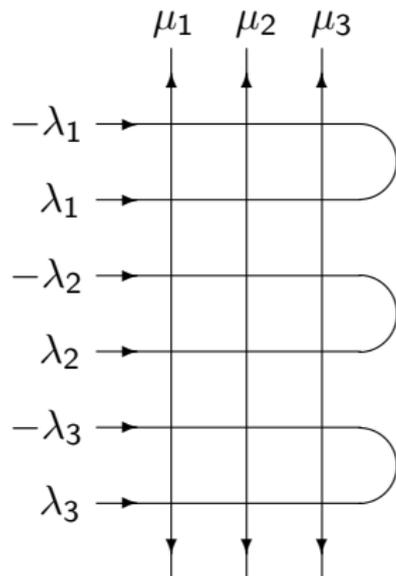# Tsuchiya partition function

In the case of open spin chains, the scalar product

$$|\phi\rangle_N = \mathcal{B}(\lambda_N)\cdots\mathcal{B}(\lambda_2)\mathcal{B}(\lambda_1)\,|\Uparrow\rangle\,.$$

leads to another partition function for the six-vertex model
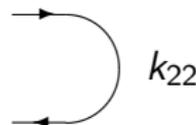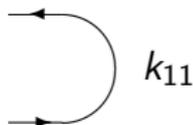
$$Z_N(\{\lambda\},\{\mu\}) = \langle\Downarrow|\,\mathcal{B}(\lambda_N)\cdots\mathcal{B}(\lambda_2)\mathcal{B}(\lambda_1)\,|\Uparrow\rangle\,.$$

# Reflecting ends

The diagonal $K$-matrix plays the role of the reflecting end,

$$K(\lambda) = \begin{pmatrix} k_{11}(\lambda) & 0 \\ 0 & k_{22}(\lambda) \end{pmatrix}.$$



$k_{11}$ $\qquad\qquad\qquad\qquad$ $k_{22}$

# Boltzmann weights

One can define the Boltzmann weights to the case $-1 < \Delta < 1$. In this case, we have

$$a(\lambda) = \sin(\gamma - \lambda), \qquad b(\lambda) = \sin(\gamma + \lambda), \qquad c(\lambda) = \sin(2\gamma),$$

where $0 < \gamma < \pi/2$ and $\Delta = -\cos(2\gamma)$.

$$k_{11}(\lambda) = \frac{\sin(\xi + \lambda + \gamma)}{\sin(\xi)}, \qquad k_{22}(\lambda) = \frac{\sin(\xi - \lambda - \gamma)}{\sin(\xi)},$$

where $\xi$ is the boundary parameter.

# Tsuchiya determinant formula - (Tsuchiya 1998)

$$
\begin{aligned}
Z_N(\{\lambda\}, \{\mu\}) &= (\sin(2\gamma))^N \prod_{i=1}^{N} \sin(2(\lambda_i + \gamma)) \frac{\sin(\xi - \mu_i)}{\sin(\xi)} \\
&\times \frac{\displaystyle\prod_{i,j=1}^{N} \sin(\gamma - (\lambda_i - \mu_j)) \sin(\gamma + \lambda_i - \mu_j) \sin(\gamma - (\lambda_i + \mu_j)) \sin(\gamma + \lambda_i + \mu_j)}{\displaystyle\prod_{\substack{i,j=1 \\ i<j}}^{N} -\sin(\lambda_j - \lambda_i) \sin(\mu_i - \mu_j) \sin(\lambda_j + \lambda_i) \sin(\mu_i + \mu_j)} \\
&\times \quad \det M,
\end{aligned}
$$

where $M$ is a $N \times N$ matrix, whose matrix elements are $M_{ij} = \phi(\lambda_i, \mu_j)$ with

$$
\phi(\lambda, \mu) = \frac{1}{\sin(\gamma - (\lambda - \mu)) \sin(\gamma + \lambda - \mu) \sin(\gamma - (\lambda + \mu)) \sin(\gamma + \lambda + \mu)}.
$$

# Homegeneous limit

- Taking $\lambda_i \to \lambda$ and $\mu_j \to \mu$.

$$
\begin{aligned}
Z_N(\lambda, \mu) &= \left[ \sin(2\gamma) \sin(2(\lambda + \gamma)) \frac{\sin(\xi - \mu)}{\sin(\xi)} \right]^N \\
&\times \frac{\left[ \sin(\gamma - (\lambda - \mu)) \sin(\gamma + \lambda - \mu) \sin(\gamma - (\lambda + \mu)) \sin(\gamma + \lambda + \mu) \right]^{N^2}}{C_N \left[ -\sin(2\lambda) \sin(2\mu) \right]^{\frac{N(N-1)}{2}}} \\
&\times \tau_N(\lambda, \mu),
\end{aligned}
$$

where $C_N = \left[ \prod_{k=1}^{N-1} k! \right]^2$. The determinant is given by

$$
\tau_N(\lambda, \mu) = \det(H),
$$

where the $H$-matrix elements are $H_{i,j} = (-\partial_\mu)^{j-1} \partial_\lambda^{i-1} \phi(\lambda, \mu)$.

# Bidimensional Toda equation (Ma 2011, Sylvester 1962)

$$-\tau_N \partial_{\mu\lambda}^2 \tau_N + (\partial_\mu \tau_N)(\partial_\lambda \tau_N) = \tau_{N+1}\tau_{N-1},$$

and can be conveniently written as

$$-\partial_{\mu\lambda}^2 [\log(\tau_N)] = \frac{\tau_{N+1}\tau_{N-1}}{\tau_N^2}, \qquad N \geq 1,$$

which is supplemented by the initial data $\tau_0 = 1$ and $\tau_1 = \phi(\lambda, \mu)$.

# Special solutions

The partition function can be cast directly in simple expressions for some special points.

$$Z_N(\lambda, \mu; \gamma = \frac{\pi}{4}) = \left( \frac{\sin(\xi \mp \mu)}{\sin(\xi)} \right)^N (\cos(2\lambda))^{\frac{N(N+1)}{2}} (\sin(2\mu))^{\frac{N(N-1)}{2}}.$$

For the cases where $\mu = \pm(\lambda + \gamma)$ and $\mu = \pm(\lambda - \gamma)$,

$$Z_N(\lambda, \pm\lambda \pm \gamma)) = \left( \frac{\sin(\xi \mp (\lambda + \gamma))}{\sin(\xi)} \right)^N (\sin(2\gamma))^{N^2} (-\sin(2\lambda))^{\frac{N(N-1)}{2}} (\sin(2(\lambda + \gamma)))^{\frac{N(N+1)}{2}},$$

$$Z_N(\lambda, \pm\lambda \mp \gamma)) = \left( \frac{\sin(\xi \mp (\lambda - \gamma)) \sin(2(\gamma + \lambda))}{\sin(\xi)} \right)^N (\sin(2\gamma))^{N^2} (\sin(2\lambda) \sin(2(\gamma - \lambda)))^{\frac{N(N-1)}{2}}.$$

The thermodynamic limit is trivial in these cases. The free energy $F = -\lim_{N \to \infty} \frac{\log(Z_N)}{2N^2}$ (we set temperature to 1) is given respectively by

$$
\begin{aligned}
e^{-2F(\lambda, \mu; \gamma = \pi/4)} &= \sqrt{\cos(2\lambda) \cos(2\mu)}, \\
e^{-2F(\lambda, \pm(\lambda + \gamma))} &= \sin(2\gamma) \sqrt{-\sin(2\lambda) \sin(2(\lambda + \gamma))}, \\
e^{-2F(\lambda, \pm(\lambda - \gamma))} &= \sin(2\gamma) \sqrt{\sin(2\lambda) \sinh(2(\gamma - \lambda))}.
\end{aligned}
$$

# VSASM

We can also fix both spectral parameters and anisotropy parameter $\gamma$, such as

$$Z_N(0, 0; \frac{\pi}{3}) = A_1^{VSASM} = \prod_{k=0}^{N-1} (3k+2) \frac{(6k+3)!(2k+1)!}{(4k+2)!(4k+3)!} = 1, 3, 26, 646, \ldots$$

which is a combinatorial point connected to the number of vertically symmetric alternating sign matrices (VSASM) due to (Kuperberg 2002)
Othe special cases are

$$Z_N(0, 0; \frac{\pi}{4}) = 2^N A_2^{VSASM} = 2^{N^2},$$

and

$$Z_N(0, 0; \frac{\pi}{6})/3^N = A_3^{VSASM} = \frac{3^{N(N-3)/2}}{2^N} \prod_{k=1}^{N} \frac{(k-1)!(3k)!}{k((2k-1)!)^2} = 1, 5, 126, \ldots,$$

where $A_x^{VSASM}$ are the $x$-enumeration of the vertically symmetric alternating sign matrices (Kuperberg 2002).

# Thermodynamic limit

$$Z_N(\lambda, \mu) = e^{-2N^2 F(\lambda, \mu) + O(N)},$$

where $F(\lambda, \mu)$ is the bulk free energy and unit temperature.
We suppose the following ansatz for the large size behaviour of the determinant $\tau_N(\lambda, \mu)$,

$$\tau_N(\lambda, \mu) = C_N e^{2N^2 f(\lambda, \mu) + O(N)},$$

where

$$e^{-2F(\lambda, \mu)} = \frac{\sin(\gamma - (\lambda - \mu)) \sin(\gamma + \lambda - \mu) \sin(\gamma - (\lambda + \mu)) \sin(\gamma + \lambda + \mu)}{\sqrt{-\sin(2\lambda) \sin(2\mu)}} e^{2f(\lambda, \mu)},$$

# Liouville equation

Substituting the ansatz in the Toda equation (1), we obtain

$$-2\partial^2_{\mu\lambda}f(\lambda,\mu) = e^{4f(\lambda,\mu)},$$

which is the Liouville equation, whose general solution has the form of

$$e^{2f(\lambda,\mu)} = \frac{\sqrt{-u'(\lambda)v'(\mu)}}{(u(\lambda)+v(\mu))},$$

for arbitrary $C^2$ functions $u(\lambda)$, $v(\mu)$.

# Solution

Our strategy is to chose $e^{2f(\lambda,\mu)}$ to match with the solution at $\gamma = \pi/4$. This leave us a $\gamma$ dependent parameter to be determined. However the $\lambda$, $\mu$ dependence was already determined.

$$e^{2f(\lambda,\mu)} = \frac{\alpha\sqrt{-\sin(\alpha\lambda)\sin(\alpha\mu)}}{\cos(\alpha\lambda) + \cos(\alpha\mu)} = \frac{\alpha\sqrt{-\sin(\alpha\lambda)\sin(\alpha\mu)}}{2\cos(\frac{\alpha}{2}(\lambda - \mu))\cos(\frac{\alpha}{2}(\lambda + \mu))} \tag{1}$$

where the parameter $\alpha = \alpha(\gamma)$ and $\alpha(\pi/4) = 4$.

# Solution (GAPR, VE Korepin, 2015)

We must use the boundary condition given by $\mu = \pm(\lambda + \gamma)$ to determine $\alpha$ parameter. In doing so we see the only possible choice for the parameter is $\alpha(\gamma) = \pi/\gamma$.

$$e^{-2F(\lambda,\mu)} = \frac{\pi \sin(\gamma - \lambda + \mu) \sin(\gamma + \lambda - \mu) \sin(\gamma - \lambda - \mu) \sin(\gamma + \lambda + \mu)}{2\gamma \sqrt{-\sin(2\lambda)\sin(2\mu)}} \frac{\sqrt{-\sin(\frac{\pi\lambda}{\gamma})\sin(\frac{\pi\mu}{\gamma})}}{\cos(\frac{\pi(\lambda-\mu)}{2\gamma})\cos(\frac{\pi(\lambda+\mu)}{2\gamma})}.$$

(2)

- ▶ The other points $\mu = \pm(\lambda - \gamma)$ are naturally fulfilled.
- ▶ As an independent check, the solution obtained also reproduces the special points $\gamma = \pi/3, \pi/4, \pi/6$.

# Ferrolectric phase: $\Delta > 1$

In the case $\Delta > 1$, one can obtain the expression for the free energy looking at the leading order state. The expression for the free energy can be written as

$$e^{-2F(\lambda,\mu)} = \sinh(\lambda - |\mu| + |\gamma|)\sqrt{\sinh(\lambda + |\mu| - \gamma)\sinh(\lambda + |\mu| + \gamma)}.$$

However due to the lack of additional boundary condition, we are unable to fix the suitable solution of Liouville equation.



$\gamma > 0$                 $\gamma < 0$
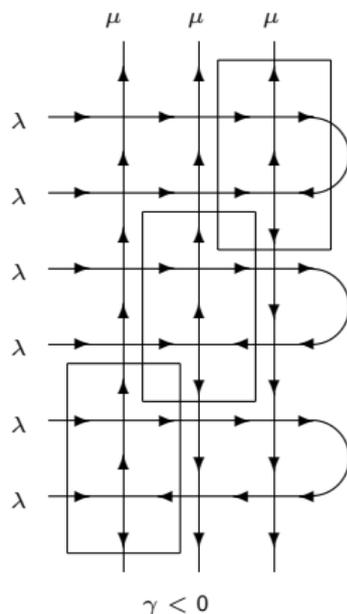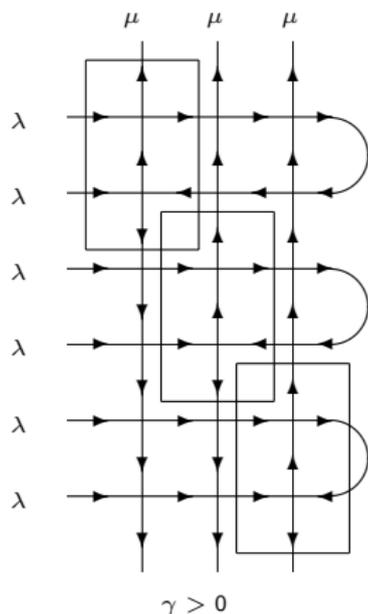
# Entropy

The number of alternating sign matrix (ASM) is given by

$$Z_N^{DWBC}(\lambda - \mu = \frac{\pi}{3}; \gamma = \frac{\pi}{3}) = A_N^{ASM} = \prod_{k=0}^{N-1} \frac{(3k+1)!}{(N+k)!} = 1, 2, 7, 42, 429, \cdots . \tag{3}$$

Taking the large limit we obtain the entropy of the six-vertex model with domain-wall boundary

$$S_{DWBC} = \frac{1}{2} \ln \left( \frac{3^3}{2^4} \right) . \tag{4}$$

The six-vertex model with reflecting end (Tsuchiya partition function) is related to the number of vertically symmetric alternating sign matrices (VSASM)

$$Z_N(0, 0; \frac{\pi}{3}) = A_1^{VSASM} = \prod_{k=0}^{N-1} (3k+2) \frac{(6k+3)!(2k+1)!}{(4k+2)!(4k+3)!} = 1, 3, 26, 646, \ldots \tag{5}$$
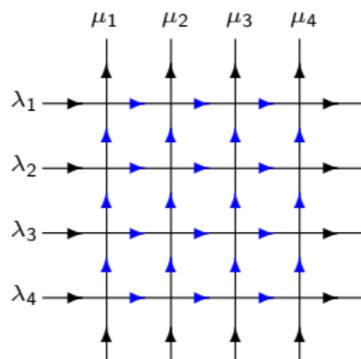
▶ Taking the large limit ($N \to \infty$) we again obtain the same value for the entropy, which means $S_{TSUCHIYA} = S_{DWBC}$.
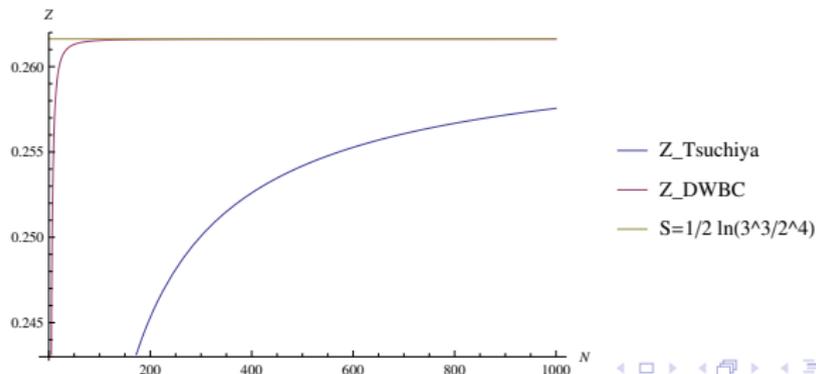
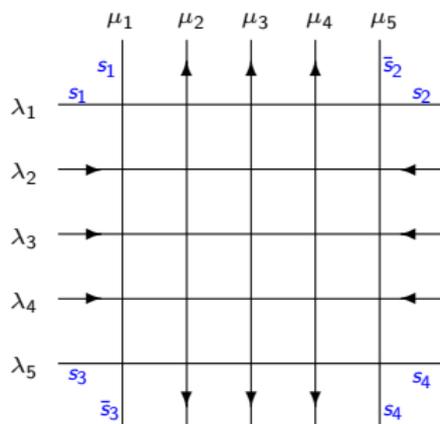# Entropy - other boundary conditions

- Ferroelectric boundary (Wu 1973)

$$Z_{FE} = 1, \tag{6}$$



$$S_{FE} = 0$$

# Entropy - other boundary conditions

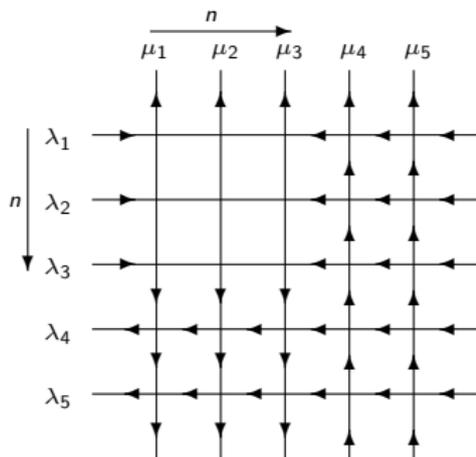▶ DWBC Descendent (TS Tavares, GAPR, VE Korepin 2015)



where $s_i = \uparrow, \downarrow$ or $\rightarrow, \leftarrow$ and $\bar{s}_i$ is its reverse.

$$S = S_{DWBC}$$

(likewise the case of reflecting end presented before.)

# Entropy - other boundary conditions

► Fusion of FE and DWBC (TS Tavares, GAPR, VE Korepin 2015)



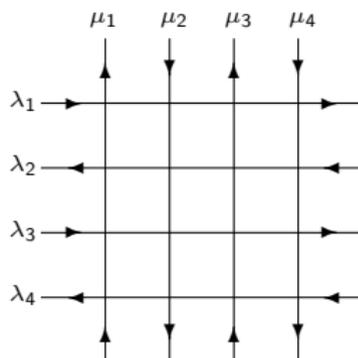$$Z_N^{fDWBC} = \prod_{ij \notin n \times n} b(\lambda_i - \mu_j) \times Z_n^{DWBC}$$

. Therefore, we see that the entropy at infinity temperature is given by

$$S_{fDWBC} = \lim_{N \to \infty} \left( \frac{n}{N} \right)^2 S_{DWBC}. \tag{7}$$

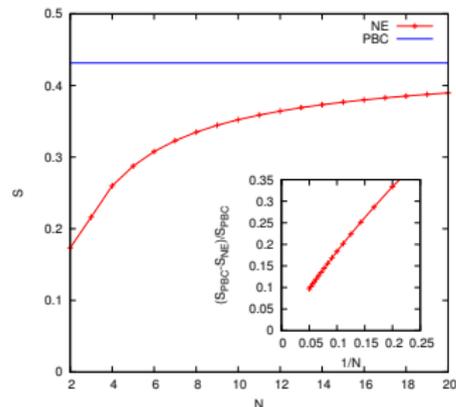$$S_{FE} \leq S \leq S_{DWBC}$$

# Entropy - other boundary conditions

▶ Néel boundary (TS Tavares, GAPR, VE Korepin 2015)



$$Z_N^{NE}(\{\lambda\}, \{\mu\}) = \langle \uparrow\downarrow \ldots \uparrow\downarrow | D(\lambda_N)A(\lambda_{N-1}) \cdots D(\lambda_2)A(\lambda_1) | \uparrow\downarrow \ldots \uparrow\downarrow \rangle,$$

$$S_{NE} = S_{PBC}(1 - \frac{\gamma}{N}),$$

where $\gamma \sim 2$.

# Entropy x boundary: six-vertex model

We believe that the entropy varies continuously in the interval,

$$S_{FE} \leq S \leq S_{PBC},$$

but we still need to compute the entropy in the $S_{DWBC} < S < S_{PBC}$.

# Concluding remarks

- We determined the free-energy in the disordered phase ($|\Delta| < 1$).

- The leading ferroelectric state was identified.

- The entropy at $a = b = c = 1$ of the six-vertex model with reflecting end was found to be the same as DWBC.

- What is the free-energy in the antiferroelectric phase?

- Is there any limiting shape curve in the case of reflecting end boundary?

Further question:

- Are there any limiting shape curves in the case of other fixed boundaries (FE/DWBC, Néel,...)

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- P.M. Bleher, V.V. Fokin, Comm. Math. Phys., 268 (2006) 223; P.M. Bleher, K. Liechty, Comm. Math. Phys. 286 (2009) 777; P.M. Bleher, K. Liechty, J. Stat. Phys. 134 (2009) 463; P.M. Bleher, K. Liechty, Comm. on Pure and Appl. Math., 63 (2010) 779.

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