# Six vertex model: Exact results and open problems

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# Problem

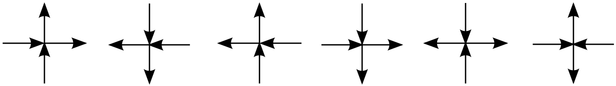
In statistical physics people believe that in thermodynamic limit the bulk free energy and correlations should not depend on boundary conditions. This is often true, but there are counterexamples.

# Six vertex model

Statistical mechanics (classical) model on a square lattice.

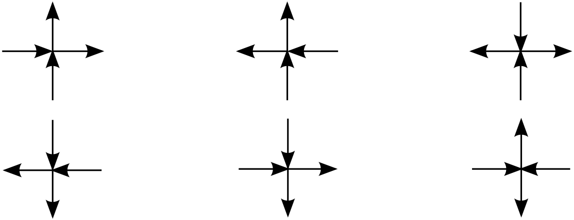
Ice model has atoms on vertices and hydrogen bonds on edges [Pauling J Am Chem Soc 1935, Slater J Chem Phys 1941].

Allowed configurations follow **arrow conservation** (ice rule).



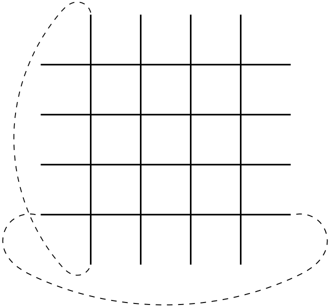
# Boltzmann weights (zero-field model)

$a = \exp(-\varepsilon_1/T)$ $\quad$ $b = \exp(-\varepsilon_2/T)$ $\quad$ $c = \exp(-\varepsilon_3/T)$



| phase | | | |
|---|---|---|---|
| FE | $a = \sinh(t-\gamma)$ | $b = \sinh(t+\gamma)$ | $c = \sinh(2\gamma)$ |
| DIS | $a = \sin(\mu-\omega)$ | $b = \sin(\mu+\omega)$ | $c = \sin(2\mu)$ |
| AFE | $a = \sinh(\lambda-\upsilon)$ | $b = \sinh(\lambda+\upsilon)$ | $c = \sinh(2\lambda)$ |

# Periodic boundary conditions (torus)



We consider here an $N \times N$ lattice.

# Partition function

$$Z = \sum_{\substack{\text{arrow} \\ \text{config.}}} \prod_{\text{vertices}} W, \qquad W \in \{a, b, c\}$$

Bulk free energy $f = -T \ln Z^{1/N^2}$, as $N \to \infty$.

Calculated by Lieb [PRL, 1967], Sutherland [PRL, 1967].
Baxter [Exactly solved models in statistical mechanics, 1982].

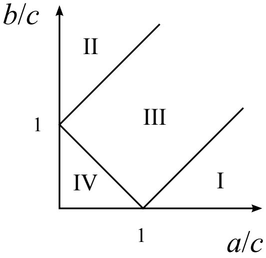
# Phases

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

Free energy has different analytic forms when

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

# Phase diagram

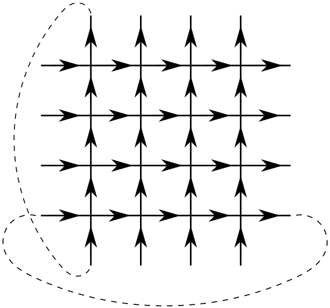



- Phase I (ferroelectric).
- Phase II (ferroelectric).
- Phase III (disordered).
- Phase IV (anti-ferroelectric).

# Phases I and II (ferroelectric)

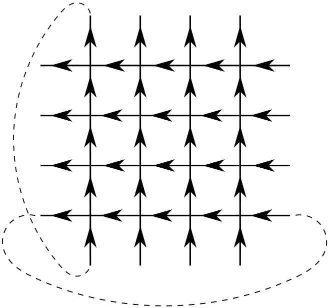
$\Delta > 1.$

Phase I:



$f = -T \ln a = \varepsilon_1$

Phase II:



$f = -T \ln b = \varepsilon_2$

No entropy in the ground state. Correlations are classical.

# Phase III (disordered)

$a, b, c < \frac{1}{2}(a+b+c)$ or $-1 < \Delta < 1$.

$$f = \varepsilon_1 - T \int_{-\infty}^{\infty} \frac{\sinh[2(\mu+\omega)x]\sinh[(\pi-2\mu)x]}{2x\sinh(\pi x)\cosh(2\mu x)}\, dx.$$

Includes infinite temperature case $(a = b = c = 1)$ where

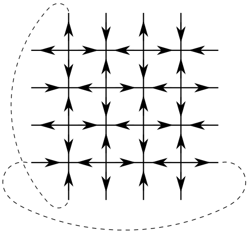
$$Z^{1/N^2} = (4/3)^{3/2}, \quad N \to \infty \text{ [Lieb PRL, 1967].}$$

Entropy of ground state.

Correlation decay as power law. Conformal field theory can be used to describe asymptotic of correlations.

# Phase IV (anti-ferroelectric)

$c > a + b$ or $\Delta < -1$.



$$f = \varepsilon_1 - T\left[(\lambda + v) + \sum_{m=1}^{\infty} \frac{e^{-2m\lambda}\sinh[2m(\lambda + v)]}{m\cosh(2m\lambda)}\right].$$

# Ferroelectric I and disordered phase III

Critical temperature $T_c$ occurs at $b + c - a = 0$.

With $(b + c - a)/a \propto T - T_c$ near critical line:

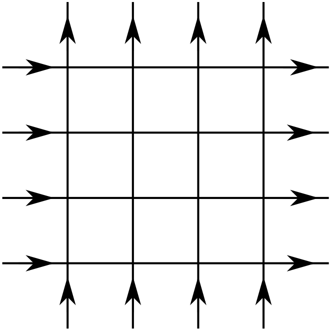
Phase transitions and critical exponents are described in detail in Baxter's book.

# Other boundary conditions

- Free boundaries.
  [Owczarek and Baxter JPA, 1989]
- Antiperiodic boundaries.
  [Batchelor, Baxter, O'Rourke, Yung JPA, 1995]

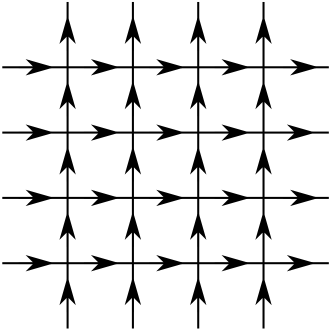
In thermodynamic limit the bulk free energy and local correlations are **identical** to periodic case.
Can the bulk free energy and correlations depend on boundary conditions in thermodynamics limit?

# Ferroelectric boundary conditions



Ferroelectric-$a$ boundary conditions.

# Ferroelectric boundary conditions

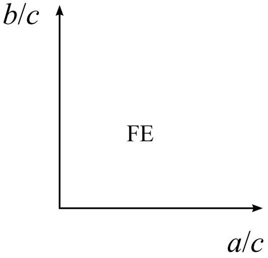


Only one arrow configuration in the bulk is compatible with these boundary conditions.

One can prove this by induction in the lattice size.

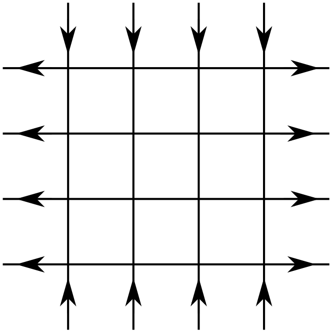
$$f = -T \ln a = \varepsilon_1$$

# Ferroelectric boundary conditions




- There are **no** phase transitions. Entropy is zero.
- One can tune Boltzmann weights into disordered phase. Correlations in the center of the lattice are pure classical. No power law, no conformal filed theory. Unlike periodic boundary conditions.
- This proves that the bulk free energy can depend on boundary conditions in thermodynamic limit.

# Domain wall boundary conditions



Korepin CMP, 1982; Korepin and Zinn-Justin JPA, 2000 [cond-mat/0004250]; Zinn-Justin PRE, 2000.

# Partition function (ferroelectric phase)

Derivation by **Bethe ansatz**.

## Izergin-Korepin formula

$$Z_N(t) = \frac{[\sinh(t+\gamma)\sinh(t-\gamma)]^{N^2}}{\left(\prod_{n=0}^{N-1} n!\right)^2}\,\tau_N(t), \quad (N \times N \text{ lattice}).$$

## Hankel determinant

$$\tau_N(t) = \det\left[\left(\frac{d}{dt}\right)^{i+k-2}\phi(t)\right], \quad \phi(t) = \frac{\sinh(2\gamma)}{\sinh(t+\gamma)\sinh(t-\gamma)}$$

# Partition function

Toda (Hirota) equation

$$\tau_N \tau_N'' - (\tau_N')^2 = \tau_{N+1}\tau_{N-1}, \quad \forall N \geq 1, \quad \tau_0 = 1, \tau_1 = \phi(t).$$

In the thermodynamic limit $N \to \infty$, use the ansatz:

$$T \ln Z_N(t) = -N^2 f(t) + \mathcal{O}(N).$$

Bulk free energy is $f(t)$.

# Free energy (ferroelectric phase)

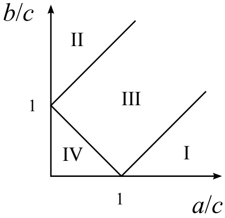
Define $f(t)/T \equiv -g(t) - \ln[\sinh(t+\gamma)\sinh(t-\gamma)]$.

**Equation and solution for $g(t)$**

$$g'' = e^{2g}, \qquad e^{g(t)} = \frac{k}{\sinh[k(t-t_0)]}.$$

with solution parameters $k$ and $t_0$.

# Phase diagram




- Phase boundaries **identical** for PBC and DWBC.
- Phases I & II (ferroelectric), III (disordered), and IV (anti-ferroelectric).

Control parameter $\Delta = \dfrac{a^2 + b^2 - c^2}{2ab} = -\cos 2\mu = -\cosh 2\lambda.$

# Ferroelectric phases I and II

$(\Delta = \cosh 2\gamma) > 1.$

**Bulk free energy**

$$e^{-f/T} = \sinh(t + |\gamma|) = \max(a, b).$$

**Same** free energy as ferroelectric phase with PBC.

- This was later rigorously proven by Bleher and Liechty, Commun. Math Phys 2009

$$Z_N = (1 - e^{-4\gamma}) \left[\sinh\left(t + |\gamma|\right)\right]^{N^2} e^{N(\gamma - 1)} (1 + O(e^{-N^{1-\epsilon}})), \forall \epsilon > 0$$

# Disordered phase III

$$-1 < (\Delta = -\cos 2\mu) < 1.$$

**Bulk free energy**

$$e^{-f/T} = \sin(\mu - \omega)\sin(\mu + \omega)\frac{\pi}{2\mu}\frac{1}{\cos(\pi\omega/2\mu)}.$$

Free energy with DWBC always **greater** than PBC case.

- This was later rigorously proven by Bleher and Fokin, Commun. Math Phys 2006

$$Z_N = C(\mu)\left(N\cos\left(\pi\omega/2\mu\right)\right)^{\kappa}\left[\frac{\pi\sin(\mu-\omega)\sin(\mu+\omega)}{2\mu\cos(\pi\omega/2\mu)}\right]^{N^2}(1+O(N^{-\epsilon}))$$

where $\kappa = \frac{1}{12} - \frac{2\mu^2}{3\pi(\pi-2\mu)}$ and $C(\mu) > 0$ is unknown.

# Entropy in disordered phase

Consider infinite temperature $a = b = c = 1$.

## Entropy with DWBC

$$S_{\text{DWBC}} = \frac{1}{2}N^2 \ln(27/16) \approx 0.26N^2.$$

## Entropy with PBC

$$S_{\text{PBC}} = \frac{3}{2}N^2 \ln(4/3) \approx 0.43N^2.$$

## Entropy with FE

$$S_{\text{FE}} = 0$$

Entropy of other boundary conditions is bounded by PBC and FE:

$$S_{FE} \leq S\text{other} \leq S_{\text{PBC}}$$

# Anti-ferroelectric phase IV with domain wall boundary conditions

$(\Delta = -\cosh 2\lambda) < -1.$

**Bulk free energy**

$$e^{-f/T} = \sinh(\lambda - v)\sinh(\lambda + v)\frac{\pi}{2\lambda}\frac{\vartheta_1'(0)}{\vartheta_2(\pi v/2\lambda)}.$$

$\vartheta_n(z)$ are Jacobi theta functions with elliptic modulus $q = e^{-\pi^2/2\lambda}$

Free energy with DWBC **different** from PBC case.
Derived by Paul Zinn-Justin.

- This was again rigorously proven by Bleher and Liechty, Commun Pure Appl Math 2010

$$Z_N = C(\lambda)[e^{-f/T}]^{N^2}\vartheta_4(N(\lambda+v)\pi/2\lambda)(1+O(N^{-1})),$$

# Ferroelectric and disordered phase III

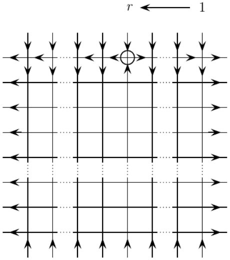
Phase transitions are in the same place
[in the space of Boltzman weights] as for periodic boundary conditions.

Critical exponents are different.

# Correlations for domain wall boundary conditions

- Boundary correlation function (determinant formula, multiple integral):
  - one-point: Bogoliubov,Pronko,Zvonarev, J PHYS A, 2002
  - two-point: Colomo, Pronko, JSTAT 2005

e.g one-point boundary correlation:




$$H_N^{(r)} = Z_N^{-1} \langle \Downarrow | B(\lambda_N) \cdots B(\lambda_{r+1}) P_\downarrow B(\lambda_r) P_\uparrow B(\lambda_{r-1}) \cdots B(\lambda_1) | \Uparrow \rangle$$

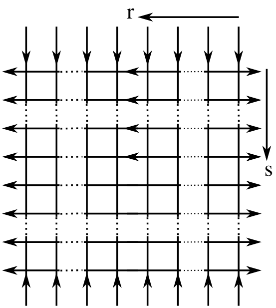
$$H_N^{(r)} = \frac{(N-1)! \sinh(2\eta)}{[\sinh(t+\eta)]^r [\sinh(t-\eta)]^{N-r+1}} \frac{\widetilde{\tau}(t)}{\tau(t)},$$

where $\tau(t) = \det(M_{ik})$ and $\widetilde{\tau}(t) = \det(\widetilde{M}_{ik})$. $\widetilde{M}_{ik}$ differs from $M_{ik} = \left(\frac{d}{dt}\right)^{i+k-2} \phi(t)$ only in the first column:

$$\widetilde{M}_{i,1} = \left(\frac{d}{d\epsilon}\right)^{i-1} \left\{ \frac{[\sinh \epsilon]^{N-r} [\sinh(\epsilon - 2\eta)]^{r-1}}{[\sinh(\epsilon + t - \eta)]^{N-1}} \right\} \Big|_{\epsilon=0}.$$

# Correlations for domain wall boundary conditions

- Emptiness formation probability EFP : Colomo, Pronko, NPB 2008




By means of orthogonal polynomials techniques, the EFP can be written as

$$F_N^{(r,s)} = \frac{(-1)^{s(s+1)/2} Z_s}{s!(2\pi i)^s a^{s(s-1)} c^s} \oint_{C_0} \cdots \oint_{C_0} \prod_{j=1}^{s} \frac{[(t^2 - 2\Delta t)z_j + 1]^{s-1}}{z_j^r (z_j - 1)^s} \times \prod_{\substack{j,k=1 \\ j\neq k}}^{s} \frac{1}{t^2 z_j z_k - 2\Delta t z_j + 1} \prod_{1\le j<k\le s} (z_k - z_j)^2 \times h_{N,s}(z_1, \ldots, z_s) h_{s,s}(u_1, \ldots, u_s)\, dz_1 \cdots dz_s,$$

where $u_j = -\frac{z_j - 1}{(t^2 - 2\Delta t)z_j + 1}$ and

$$h_{N,s}(z_1, \ldots, z_s) = \prod_{\substack{i,j=1 \\ i<j}}^{s} \frac{1}{z_j - z_i} \det\left(z_k^{s-i}(z_k - 1)^{i-1} h_{N-s+i}(z_k)\right),$$

$h_N(z)$: generating function of $H_N^{(r)}$ ($h_N(z) = \sum_{r=1}^{N} H_N^{(r)} z^{r-1}$).

# Artic curve: spatial phase separation

This curve separates the ferroelectric and the disordered phases.

- $\Delta = 0$: Artic circle (Elkies, Kuperberg, Larsen, Propp, J Algebraic Combin, 1992)

$$(2x-1)^2 + (2y-1)^2 = 1$$

- $\Delta \to -\infty$: rectangle (Zinn-Justin PRE 2000)

- $\Delta = \frac{1}{2}$: ellipse describes the limit shape of alternating sign matrix (Colomo, Pronko SIAM J Discrete Math, 2010)

$$(2x-1)^2 + (2y-1)^2 - 4xy = 1$$

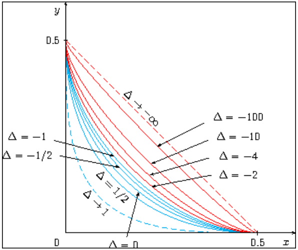
- $\Delta = -\frac{1}{2}$: algebraic equation of sixth order

$$\begin{aligned} &324(x^6+y^6) + 1620(x^5y+xy^5) + 3429(x^4y^2+x^2y^4) + 4254x^3y^3 - 972(x^5+y^5) \\ &- 1458(x^4y+xy^4) - 2970(x^3y^2+x^2y^3) - 6147(x^4+y^4) - 9150(x^3y+xy^3) - 17462x^2y^2 \\ &+ 13914(x^3+y^3) + 24086(x^2y+xy^2) - 11511(x^2+y^2) - 17258xy + 4392(x+y) - 648 = 0. \end{aligned}$$

# Artic curve: spatial phase separation

- Taking the scaling limit of EFP $(N, r, s \to \infty$, such that $x = r/N$ and $y = s/N$ ) in the saddle-point approximation: Colomo,Pronko, J STAT PHYS 2010, Colomo,Pronko, Zinn-Justin, JSTAT 2010

$-1 \leq \Delta < 1$ (disordered)




$$x = \frac{\varphi'(\zeta+\eta)\Psi(\zeta) - \varphi(\zeta+\eta)\Psi'(\zeta)}{\varphi(\zeta+\lambda)\varphi'(\zeta+\eta) - \varphi(\zeta+\eta)\varphi'(\zeta+\lambda)},$$
$$y = \frac{\varphi(\zeta+\lambda)\Psi'(\zeta) - \varphi'(\zeta+\lambda)\Psi(\zeta)}{\varphi(\zeta+\lambda)\varphi'(\zeta+\eta) - \varphi(\zeta+\eta)\varphi'(\zeta+\lambda)}.$$

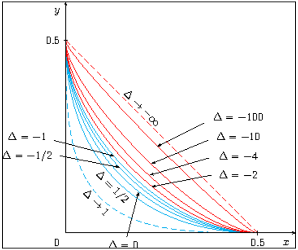
$$\varphi(\zeta) = \frac{\sin 2\eta}{\sin(\lambda-\eta)\sin(\lambda+\eta)},$$
$$\Psi(\xi) = \cot\xi - \cot(\xi+\lambda+\eta) - \alpha\cot(\alpha\xi) + \alpha\cot\alpha(\xi+\lambda-\eta).$$

where $\alpha = \pi/(\pi - 2\eta)$ and $\zeta \in [0, \pi - \lambda - \eta]$.

# Artic curve: spatial phase separation

- Taking the scaling limit of EFP $(N, r, s \to \infty$, such that $x = r/N$ and $y = s/N$ ) in the saddle-point approximation: Colomo,Pronko, J STAT PHYS 2010, Colomo,Pronko, Zinn-Justin, JSTAT 2010

$-\infty < \Delta < -1$ (antiferroelectric)




$$x = \frac{\varphi'(\zeta-\eta)\Psi(\zeta) - \varphi(\zeta-\eta)\Psi'(\zeta)}{\varphi(\zeta+\lambda)\varphi'(\zeta-\eta) - \varphi(\zeta-\eta)\varphi'(\zeta+\lambda)},$$

$$y = \frac{\varphi(\zeta+\lambda)\Psi'(\zeta) - \varphi'(\zeta+\lambda)\Psi(\zeta)}{\varphi(\zeta+\lambda)\varphi'(\zeta-\eta) - \varphi(\zeta-\eta)\varphi'(\zeta+\lambda)}.$$

$$\varphi(\zeta) = \frac{\sinh 2\eta}{\sinh(\eta-\lambda)\sinh(\eta+\lambda)},$$

$$\Psi(\zeta) = \coth\zeta - \coth(\zeta+\lambda-\eta) - \alpha\frac{\vartheta_1'(\alpha\zeta)}{\vartheta_1(\alpha\zeta)} + \alpha\frac{\vartheta_1'(\alpha(\zeta+\lambda+\eta))}{\vartheta_1(\alpha(\zeta+\lambda+\eta))}$$

where $\alpha = \pi/2\eta$ and $\zeta \in [0, \eta-\lambda]$.
Comment: algebraic curve in roots of unit cases; transcendent elsewhere.

# Open problems

- Classification of boundary conditions into universality classes: corresponding to given entropy [in thermodynamic limit].
- Prove that the bulk free energy is the same for b.c. in one universality class.
- Prove that for majority of b. c. the phase boundaries are the same as for periodic case [in the space of Boltzman weights].
- Prove that evaluation of the partition function for majority of boundary conditions are NP hard.
- Find new boundary conditions for which the model is exactly solvable.
- Describe behavior of correlations across the arctic circle. How quantum corrections turn into classical.

# Summary

- Six vertex model was discovered in 1935. We learned a lot about the model, but there open problems.

# References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6. F Colomo and AG Pronko, J STAT PHYS, **138**, 662 (2010).
7. F Colomo, AG Pronko and P Zinn-Justin J STAT MECH, L03002 (2010).