Six vertex model: Exact results and open problems

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Problem

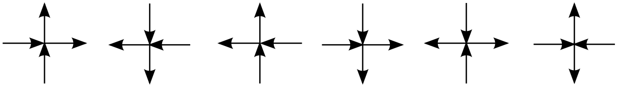
In statistical physics people believe that in thermodynamic limit the bulk free energy and correlations should not depend on boundary conditions. This is often true, but there are counterexamples.

Six vertex model

Statistical mechanics (classical) model on a square lattice.

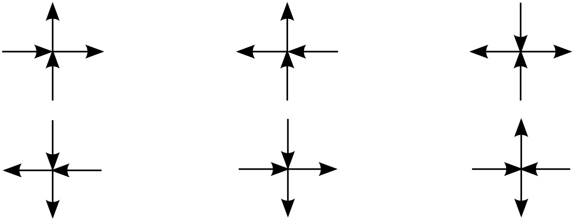
Ice model has atoms on vertices and hydrogen bonds on edges [Pauling J Am Chem Soc 1935, Slater J Chem Phys 1941].

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



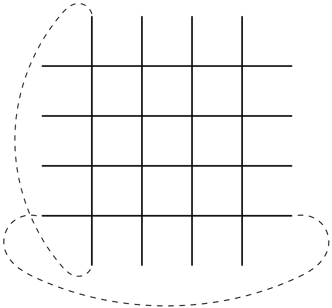
Boltzmann weights (zero-field model)

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



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].

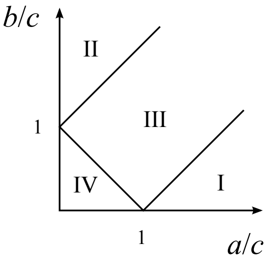
Phases

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

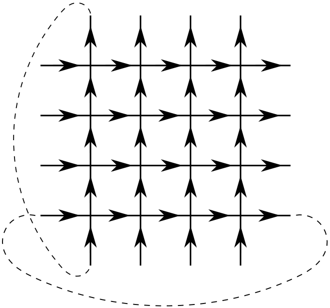


- Phase I (ferroelectric).
- Phase II (ferroelectric).
- Phase III (disordered).
- Phase IV (anti-ferroelectric).

Phases I and II (ferroelectric)

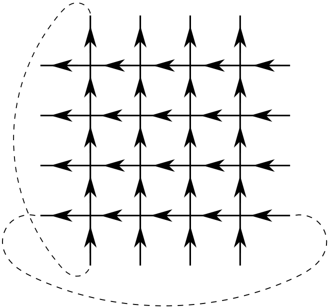
$\Delta > 1.$

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

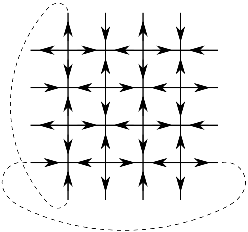
$$Z^{1/N^2} = (4/3)^{3/2}, \quad N \to \infty \text{ [Lieb PRL, 1967].}$$

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 $b + c - a = 0$. ($2\mu \to \pi$ and $2w \to -\pi$)

With $\theta = (b + c - a)/a \propto T - T_{\text{c}}$ near critical line:

- $\theta \approx \frac{1}{2}(\pi - 2\mu)(\mu + \omega)$ as $\theta \to 0^+$.
- Free energy f is **continuous** at $\theta = 0$.
- Critical exponent for specific heat $\alpha = 1$ (step discontinuity).
- Phase transition is **first-order**.
- Correlation length is zero in ferroelectric phase and infinite in disordered phase.

Ferroelectric II and disordered phase III

Same as previous ferroelectric I–disordered phase transition with:

- $a \leftrightarrow b$.
- Phase I $\leftrightarrow$ Phase II.
- Corresponds to $\pi/2$ rotation of lattice.

Anti-ferroelectric IV and disordered phase III

Critical temperature T_{c} occurs at $a+b-c=0$. $(\lambda, v \to 0^+)$

- $\theta \approx \frac{1}{2}(v^2-\lambda^2)$ as $\theta \to 0^-$.
- Free energy is **singular** as $\theta \to 0^-$:

$$f_{\mathsf{c}} \propto e^{-\pi^2/2\lambda} \sim e^{-\mathsf{const}/|\theta|^{1/2}}, \quad (\mathsf{const}\ > 0).$$

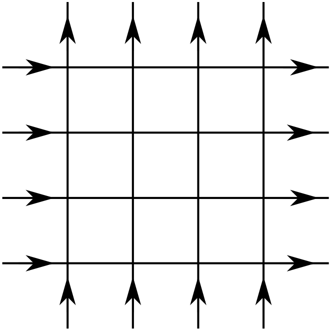
- All temperature derivatives of f are continuous at $\theta = 0$.
- Phase transition is **infinite-order**.
- Inverse correlation length $\xi^{-1} \propto f_{\mathsf{c}}^{1/2}$ also singular as $\theta \to 0^-$. Correlation length does not diverge as a power law.

Other boundary conditions

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

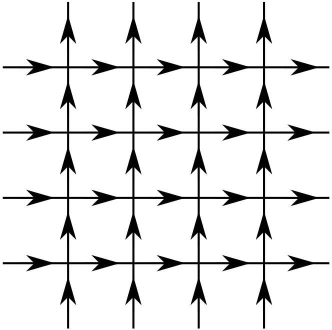
In thermodynamic limit the bulk free energy and correlations are **identical** to periodic case.
Can the bulk free energy and correlations depend on boundary conditions in thermodynamics limit?

Ferroelectric boundary conditions



Ferroelectric-a boundary conditions.

Ferroelectric boundary conditions

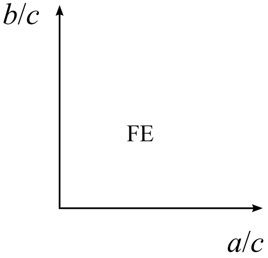


Only one arrow configuration in the bulk is compatible with these boundary conditions.

One can prove this by induction in the lattice size.

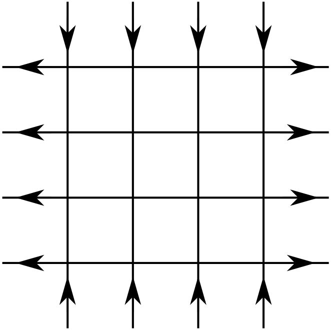
$$f = -T \ln a = \varepsilon_1$$

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)

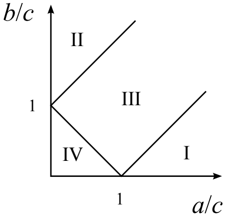
Define $f(t)/T \equiv -g(t) - \ln[\sinh(t+\gamma)\sinh(t-\gamma)]$.

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

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

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

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

Entropy with PBC

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

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

Let $\theta \propto (T/T_{\mathsf{c}}) - 1$.

- Free energy f is **continuous** at $\theta = 0$.
- Specific heat $\sim \theta^{1/2}$ in disordered phase $\theta \to 0^+$.
  Critical exponent $\alpha = -1/2$
  ($\alpha = 1$ for PBC).
- Phase transition is **second-order**
  (first-order for PBC).

Anti-ferroelectric IV and disordered phase III

Phase transition reached as $\lambda, v \to 0$.

Leading singularity of free energy is

$$f_{\mathsf{c}} \sim e^{-\pi^2/\lambda}.$$

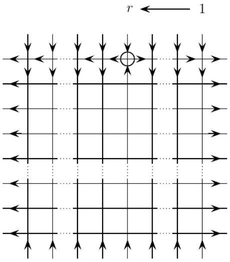
Let $\theta \propto (T/T_{\mathsf{c}}) - 1$.

- Like in PBC case $f_{\mathsf{c}} \propto e^{-\mathsf{const}/|\theta|^{1/2}}$ as $\theta \to 0^-$.
- Phase transition is also **infinite-order**.

Correlations for domain wall boundary conditions

- No results for bulk correlation function
- 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:



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

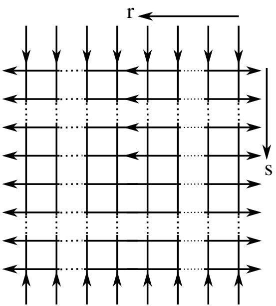
$$H_N^{(r)} = \frac{(N-1)! \sinh(2\eta)}{[\sinh(t+\eta)]^r [\sinh(t-\eta)]^{N-r+1}} \frac{\widetilde{\tau}(t)}{\tau(t)},$$

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 (introduced by Korepin 1988): 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 $H_N^{(r)}$ $(h_N(z) = \sum_{r=1}^{N} H_N^{(r)} z^{r-1})$.

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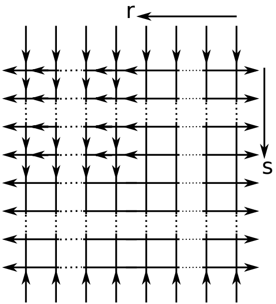

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where $u_j = -\frac{z_j - 1}{(t^2 - 2\Delta t)z_j + 1}$ and

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

$h_N(z)$: 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)

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

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

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

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

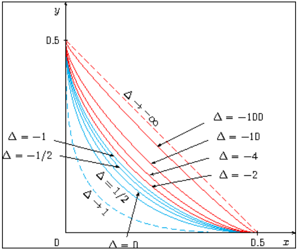
- $\Delta = -\frac{1}{2}$: algebraic equation of sixth order

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

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)



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

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

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

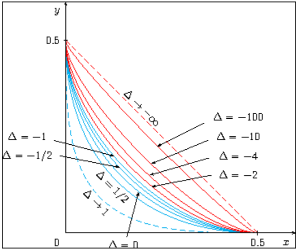
$$\Psi(\xi) = \cot\xi - \cot(\xi+\lambda+\eta) - \alpha\cot(\alpha\xi) + \alpha\cot\alpha(\xi+\lambda-\eta).$$

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: describe all boundary conditions corresponding given entropy [in thermodynamic limit].
- Prove that the bulk free energy is the same for all boundary conditions in one universality class.
- Prove that for majority of boundary conditions 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.

Summary

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

References

1. V Korepin, CMP, vol 86, page 361 (1982).
2. V Korepin and P Zinn-Justin JPA **33**, 7053 (2000); cond-mat/0004250.
3. P Zinn-Justin PRE **62**, 3411 (2000).
4. R J Baxter *Exactly solved models in statistical mechanics* (AP, London, 1982).
5. V E Korepin, N M Bogoliubov, and A G Izergin *Quantum inverse scattering method and correlation functions* (CUP, Cambridge, 1993).
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).