Percolation, polymers and square ice: exact formulas and finite size scaling.

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Motivation

- Percolation gives the simplest example of continuous phase transition that describes the change of global connectivity in a large random system.
- Most of the results available are obtained for the infinite system or in the thermodynamic limit. Can one obtain finite size results?
- Critical bond percolation on 2D square lattice is related to the integrable six-vertex model at the so-called Razumov-Stroganov combinatorial (stochastic) point known for a peculiar combinatorial structure of model observables.
- The idea is to use the toolbox of the theory of quantum integrable systems, like Bethe ansatz and T-Q Baxter equation, to solve the finite size systems .

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Outline

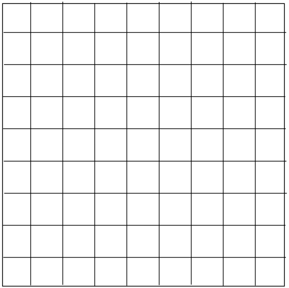
Origins of percolation theory (Broadbent 1954, Broadbent and Hammersley 1957)

Broadbent was at that time working at the British Coal Utilization Research Association on the design of gas masks for use in coal mines. These masks contained porous carbon granules into which the gas could penetrate. The pores in a granule constituted a random network of tiny interconnecting tunnels, along which the gas could move by surface adsorption. If the pores were large enough and richly enough connected, the gas could permeate the interior of a granule; but, if the pores were too small or inadequately connected, the gas would not get beyond the outer surface of the granules. Thus there was a critical point, above which the mask worked well and below which it was ineffective.

(Hammersly 1983, from B.D. Hughes, Random walks and random environments)

Bond percolation

- Consider a graph (lattice).
- Every bond of the graph is chosen to be either open (thick) with probability p or closed (thin) with probability $(1-p)$. Open bonds sharing a vertex belong to the same connected cluster.



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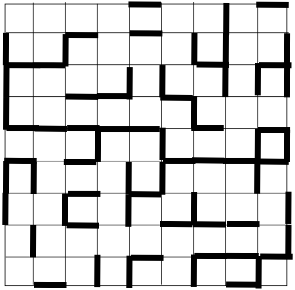

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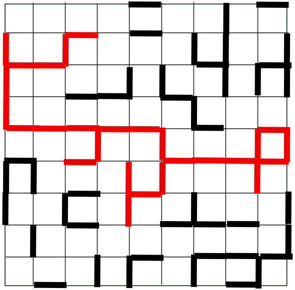

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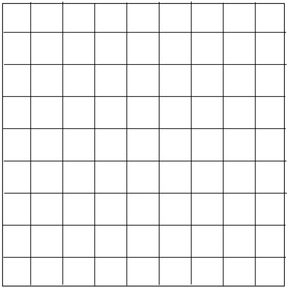

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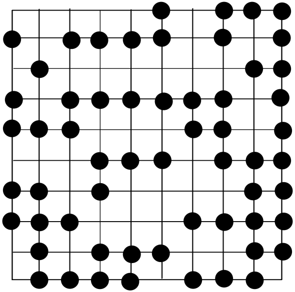

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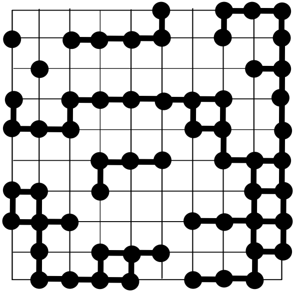

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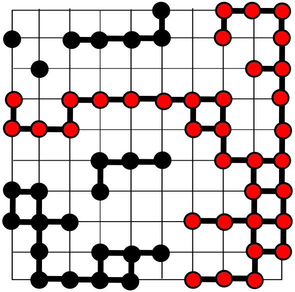

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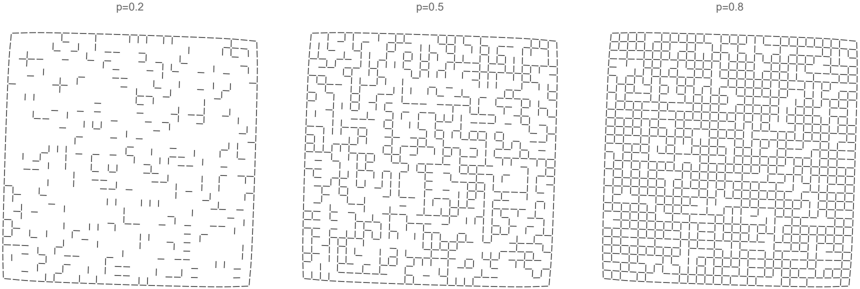
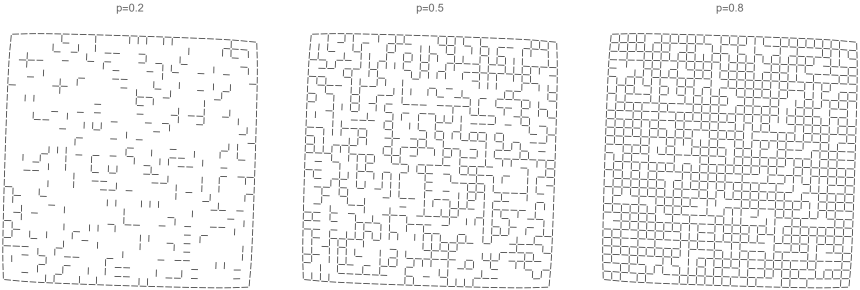
Percolation at an infinite lattice



Percolation at an infinite lattice

- At $p = 0$ the lattice is empty (no clusters). At $p = 1$ all sites belong to a single infinite cluster with probability one. Probability $P_\infty = \mathbb{P}[\text{there is an infinite cluster}]$ is a non-decreasing function of p.



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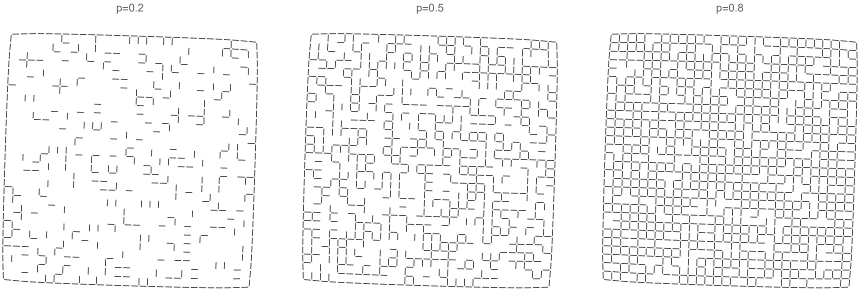


- There is a critical point $p_c \in [0, 1]$, such that $P_\infty = 0$ when $p < p_c$, and $P_\infty = 1$ when $p > p_c$. In the latter case on translation invariant d-dimensional lattices there is exactly one infinite cluster with probability one.

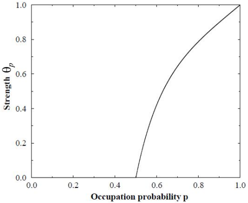
Percolation threshold

Lattice	# nn	Site percolation	Bond percolation
1d	2	**1**	**1**
2d Honeycomb	3	0.6962	$1-2\sin(\pi/18) \approx 0.65271$
2d Square	4	**0.592746**	**1/2**
2d Triangular	6	**1/2**	$2\sin(\pi/18) \approx 0.34729$
3d Diamond	4	0.43	0.388
3d Simple cubic	6	0.3116	0.2488
3d BCC	8	0.246	0.1803
3d FCC	12	0.198	0.119
4d Hypercubic	8	0.197	0.1601
5d Hypercubic	10	0.141	0.1182
6d Hypercubic	12	0.107	0.0942
7d Hypercubic	14	0.089	0.0787
Bethe lattice	z	**1/(z-1)**	**1/(z-1)**

Percolation threshold for various lattices in various dimensions.
(Christensen, K. (2002). Percolation theory.)

Percolation as a continuous phase transition

Order parameter:
Strength $\theta_p = \mathbb{P}$[a site belongs to an infinite cluster]



Critical exponents, $p \to p_c$:
α : the density of clusters $\nu_c = A + B(p-p_c) + C(p-p_c)^2 + D_\pm |p-p_c|^{2-\alpha} + \cdots$;
β : order parameter decay $\theta_p \sim (p-p_c)^\beta$;
γ : mean cluster size $S \sim |p-p_c|^{-\gamma}$
ν: $g(\mathrm{r}) = \mathbb{P}$[two sites on the distance r are connected] $\asymp e^{-\frac{|r|}{\xi}}, \xi \sim |p-p_c|^{-\nu}$.
η : connectivity at the critical point $p = p_c$, $g(\mathrm{r}) = |r|^{2-d-\eta}$
τ, σ : cluster size distribution $n_s \sim s^{-\tau} e^{\frac{s}{s_\xi}}$, size cutoff $s_\xi \sim |p-p_c|^{-1/\sigma}$
D : fractal dimension $s_\xi \sim \xi^D$

Critical exponents:

Exponent	**1d**	**2d**	3d	4d	5d	6d	**Bethe**
α	1	$-2/3$	-0.62	-0.72	-0.86	-1	-1
β	**0**	5/36	0.41	0.64	0.84	1	**1**
γ	**1**	43/18	1.80	1.44	1.18	1	**1**
ν	**1**	**4/3**	0.88	0.68	0.57	1/2	**1/2**
σ	**1**	36/91	0.45	0.48	0.49	1/2	**1/2**
τ	**2**	**187/91**	2.18	2.31	2.41	5/2	**5/2**
$D(p = p_c)$	**1**	**91/48**	2.53	3.06	3.54	4	**4**

Percolation critical exponents in dimensions $d = 1; 2; 3; 4; 5; 6$ and in the Bethe lattice. *(Christensen, K. (2002). Percolation theory.)*

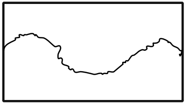
The critical exponents vary with dimension d, when d is less than the upper critical

$$d_c = 6.$$

As usual, when $d \geq d_c$, the mean field theory is exact.

Conformal invariance in 2D.

- In two dimensions, $d = 2$, the critical percolation at $p = p_c$ is believed to possess conformal invariance in continuous limit. (Proved for site percolation on triangular lattice, Smirnov, 2009.) The conformal invariance suggests that the theory can be described in terms of exactly solvable conformal field theory, which makes all the correlation functions accessible, at least potentially.



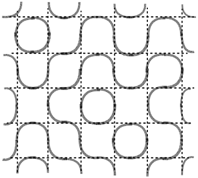
crossing probability

- Consequences of conformal invariance for critical systems in finite geometry are the universal finite size corrections to physical quantities.

  Free energy on the cylinder of circumference L: $f_L = f_\infty - \frac{\pi c}{6} L^{-2}$, where c is the central charge of the theory. For critical percolation $c = 0$. The observables are derivative of f_L with respect to conjugated fields, which can change the value of c. Hence, we expect universal finite size correction for percolation observables in a finite size system.

O(n) dense loop model on square lattice

- A path passes through every bond exactly once, and two paths meet at every site without crossing each other. Every closed loop is given weight n. We are interested in the stochastic case $n = 1$.



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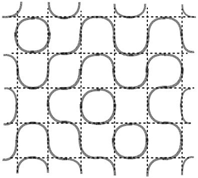
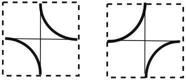


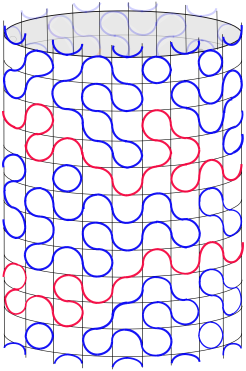
- To construct configurations by local operations we place a vertex at every lattice site, in which two pairs of paths at four incident bonds are connected pairwise in one of two possible ways



For $n = 1$ these vertices have equal weights.

O(n) dense loop model on a cylinder

- Consider a strip of the square lattice of even width $L = 2N$ wrapped into a cylinder



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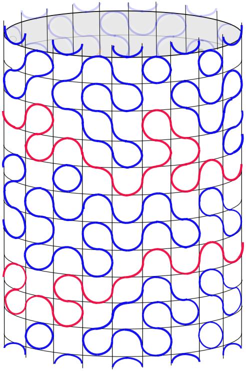

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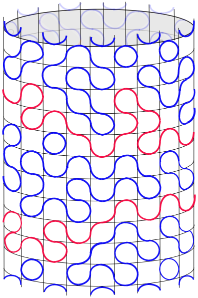
- $\nu_c(L)$ – density of contractible loops
  $\nu_{nc}(L)$ – density of non-contractible loops

From O(1) dense loop model to critical percolation



- Construct the 45° rotated square lattice with vertices in odd-odd and even-even faces.
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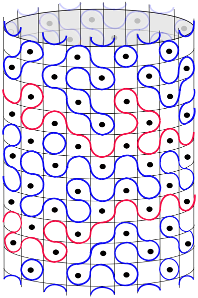

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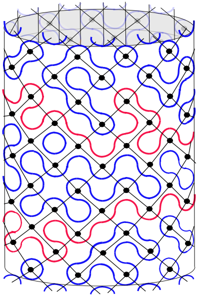

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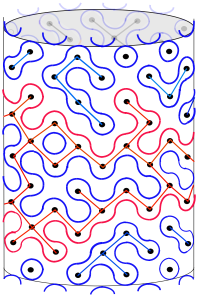

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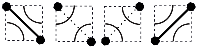
- The O(1) Gibbs measure on loops induces the critical $(p = 1/2)$ measure on percolation clusters by identification  .

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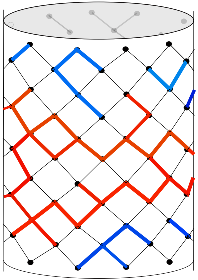

- Construct the 45° rotated square lattice with vertices in odd-odd and even-even faces.
- The O(1) Gibbs measure on loops induces the critical $(p = 1/2)$ measure on percolation clusters.
- Cluster densities coincide with the loop densities
  $\nu_c(L)$ – density of clusters that do not wrap around the cylinder
  $\nu_{nc}(L)$ – density of clusters wrapping around the cylinder

Previous results

- Infinite plane limit (Temperley, Lieb 1971, Ziff, Finch, Adamchik 1997)

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  - For O(n) dense loop model (Brankov, Priezzhev, Rittenberg, Rogozhnikov 2014) from Bethe ansatz solution of XXZ model and CFT (Alcaraz, Barber, Batchelor 1988; Quispel, Batchelor, 1987; Destri, De Vega 1989;von Gehlen, Rittenberg 1987)

$$v_{nc}(L) = \frac{1}{\sqrt{3}L^2} + O(1/L^3), \quad v_c(L) = v(\infty) + \frac{1}{4\sqrt{3}L^2} + O(1/L^3)$$

Results. Loop (cluster) densities for arbitrary even $L = 2N$. Contractible loops. **(A.P. 2021)**

- Exact formula

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\begin{aligned}
v_c(2N) &= \frac{3\Gamma\left(\frac{N}{2}\right)\Gamma\left(\frac{3N}{2}+\frac{1}{2}\right)}{4\Gamma\left(\frac{3N}{2}\right)\Gamma\left(\frac{N+1}{2}\right)} + \frac{\pi^2 2^{-2N} 3^{2-3N}\Gamma(3N)}{\Gamma\left(\frac{N}{2}+\frac{1}{6}\right)^2\Gamma\left(\frac{N}{2}+\frac{5}{6}\right)^2\Gamma(N)} - \frac{5}{2} \\
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- Asymptotic expansion

$$\nu_c(2N) = \frac{3\sqrt{3}-5}{2} + \frac{1}{4\sqrt{3}}(2N)^{-2} - \frac{23}{48\sqrt{3}}(2N)^{-4} + O\left(N^{-6}\right).$$

Results. Loop (cluster) densities for arbitrary even $L = 2N$. Non-contractible loops. **(A.P. 2021)**

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$$\nu_{nc}(2N) = \frac{2^{2(N-2)}\Gamma(N)}{N\pi^2\Gamma(3N)} \left(3^{3N}\Gamma\left(\frac{N}{2}+\frac{1}{6}\right)^2\Gamma\left(\frac{N}{2}+\frac{5}{6}\right)^2 - \frac{12\pi^2\Gamma\left(\frac{3N}{2}\right)^2}{\Gamma\left(\frac{N}{2}\right)^2}\right)$$
$$= \frac{1}{8}, \frac{11}{320}, \frac{421}{26880}, \frac{1403}{157696}, \frac{4189}{732160}, \frac{952067}{238977024}, \ldots$$

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$$v_{nc}(2N) = \frac{1}{\sqrt{3}}(2N)^{-2} - \frac{17}{18\sqrt{3}}(2N)^{-4} + \frac{1021}{216\sqrt{3}}(2N)^{-6} + O\left(N^{-8}\right).$$

Transfer matrix of O(1) DLM model

- Construct O(1) DLM configurations on the cylinder layer by layer acting with the transfer matrix.
- Consider a vector space spanning the basis consisting of vectors indexed by partial non-crossing pairings of L points on the outer boundary of annulus (pairings depicted by chords + defects linking a point to infinity).
- Action of O(1) DLM transfer matrix converts basis vectors to basis vectors (pairings to pairings) by rewiring the links
- Up to a normalization by the factor 2^L the trasfer matrix is the transition matrix of a Markov chain. Its largest eigenvalue is $\Lambda_0^{DLM} = 2^L$ is non-degenerate and corresponds to the stationary state eigenvector with non-negative components.

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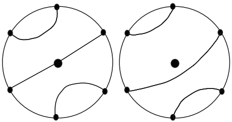

- Action of O(1) DLM transfer matrix converts basis vectors to basis vectors (pairings to pairings) by rewiring the links
- Up to a normalization by the factor 2^L the trasfer matrix is the transition matrix of a Markov chain. Its largest eigenvalue is $\Lambda_0^{DLM} = 2^L$ is non-degenerate and corresponds to the stationary state eigenvector with non-negative components.

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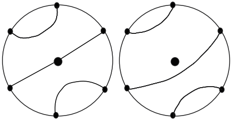

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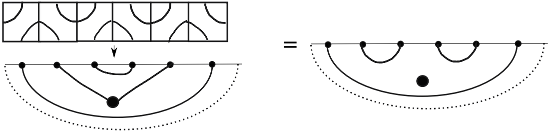

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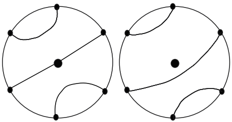

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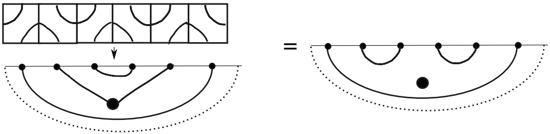

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Stationary state

- Stationary state eigenvector

$$\mathscr{L}\Psi_L = 2^L \Psi_L$$

- Stationary state is a linear combination of the perfect non-crossing pairings

Stationary states of the O(1) DLM for $L=4$

- Stationary state eigenvector has a rich combinatorial content (*Razumov, Stroganov, 2001*). The probability normalization equals to the number half turn symmetric ASM (*GNPR, 2002; Di Francesco, Zinn-Justin, Zuber 2006*):

$$A_{\mathrm{HT}}(L) = \prod_{k=0}^{L/2-1} \frac{(3k+2)!(3k)!}{(L/2+k)!^2},$$

and the components contain their refined enumeration.

- The average stationary state observables are expected to be given by rational numbers. Can one use the toolbox of integrable systems to calculate them?

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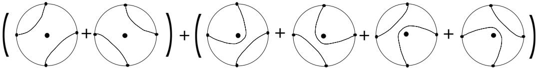
$\Psi_4 = 3$



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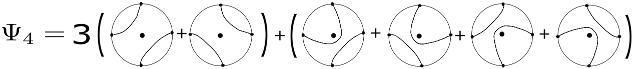

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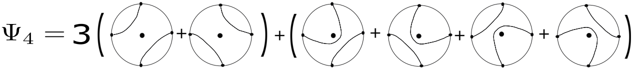

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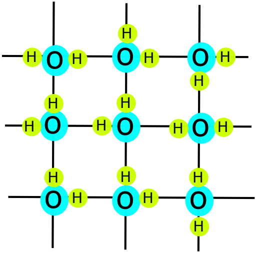
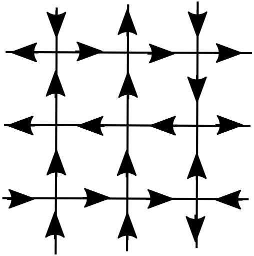
Residual entropy of square ice.

Haw many ways are there to arrange the molecules H_2O of water on the square lattice.





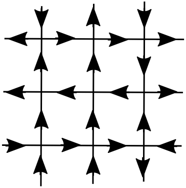
$$S = kN \ln W$$

Linus Pauling (1935): $W \simeq \frac{3}{2} = 1.5$

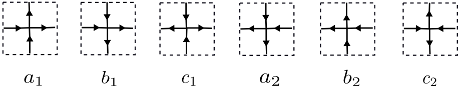
Elliot Lieb (exact, 1967): $W = \left(\frac{4}{3}\right)^{\frac{3}{2}} \simeq 1.5396$

Six-vertex model

Six vertex model is a probability distribution on the set $\Omega(\mathscr{L})$ of compatible arrow configurations on a domain $\mathscr{L}$ of the square lattice:



$$\mathbb{P}(\omega) = \frac{W(\omega)}{Z_{\mathscr{L}}}$$



Statistical (Boltzmann) weight of an arrow configuration :

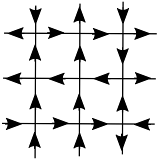
$$W(\omega) = a_1^{\#(a_1)} \dots c_2^{\#(c_2)}$$

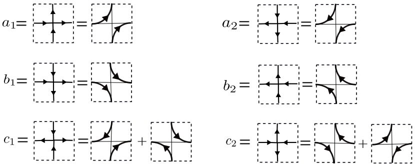
Partition function:

$$Z_{\mathscr{L}}^{6V} = \sum_{\omega \in \Omega(\mathscr{L})} W(\omega)$$

From loops to six-vertex model (Baxter,Kelland,Wu 1976)

Six-vertex model $\xleftarrow{\text{sum over connectivities}}$ Directed loop model $\xrightarrow{\text{sum over directions}}$ Loop model





Let us set $\quad a_1 = b_1 = u^{1/2}, a_2 = b_2 = u^{-1/2}, c_1 = c_2 = q^{1/2} + q^{-1/2}.$

Then, the weights of contractible and non-contractible loops on an infinite cylinder of even circumference L are

$$n = 2_q = q + q^{-1} \quad \text{and} \quad v = u^{L/2} + u^{-L/2},$$

Let $\mathscr{L}$ be an $L \times K$ rectangular domain with periodic boundary conditions (torus with periods L, K). The per-site free energies of Dense Loop Model and Six-Vertex model on the infinite cylinder obtained in the limit $K \to \infty$ coincide:

$$f_L(n,v) = \lim_{K\to\infty} \frac{1}{KL} \ln Z^{6V}_{L,K}(q,u) = \lim_{K\to\infty} \frac{1}{KL} \ln Z^{DLM}_{L,K}(n,v).$$

From loops to six-vertex model

- The Dense loop-Six Vertex correspondence ensures the contractible and non-contractible loop weights

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$$q = u^{L/2} = e^{\mathrm{i}\frac{\pi}{3}}$$

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$$q = u^{L/2} = e^{\mathrm{i}\frac{\pi}{3}}$$

- Loop densities are derivatives of the free energy

$$\nu_c(L) = n \frac{d}{dn}\bigg|_{n=1} f_L(n,1), \quad \nu_{nc}(L) = v \frac{d}{dv}\bigg|_{v=1} f_L(1,v)$$

Steps of solution

- Construct transfer-matrix of the six vertex model. The free energy is given by its largest eigenvalue.
- Diagonalize the transfer-matrix by the Bethe ansatz. $\Rightarrow$ Bethe equations.
- Reformulate Bethe equations into T-Q, T-P functional equations.
- At the Razumov-Stroganov point T-Q, T-P equations are reduced to a single difference equation solved in terms of the hypergeometric functions (Fridkin, Stroganov, Zagier 2000,2001). $\Rightarrow$ The largest eigenvalue.
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O(1) DLM on cylinder of odd circumference

- Since no perfect matching of an odd number of points is possible, at least one infinite defect exists in any configuration of O(1) DLM at a cylinder of even circumference. Hence, no non-contractible loops are present.

- The stationary state of the associated Markov chain contains only configurations with a single defect and all other sites paired.
- The largest eigenvalue of the associated six-vetex model is twice degenerate with eigenstates belonging to the invariant subspaces $\mathscr{H}_M$ with $M = (L \pm 1)/2$. Under spin-link correspondence they are interpreted as the link states with directed defects.

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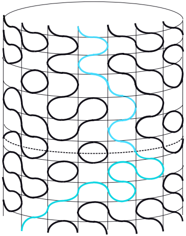

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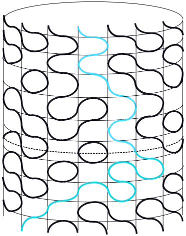

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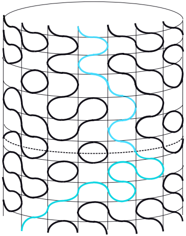

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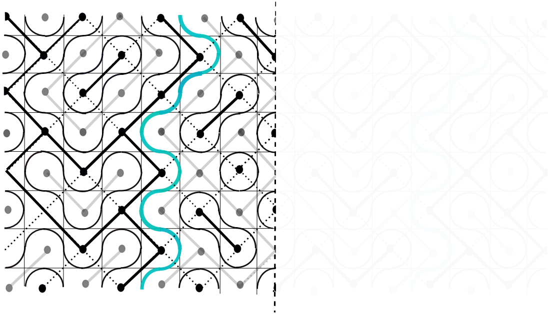
O(1) DLM on cylinder of odd circumference and percolation



Correspondence between the configuration of the $O(1)$ loop model (pictured twice side-by-side in thin black solid lines with the defect line shown in blue) and the associated percolation cluster (thick solid black lines) on the rotated lattice. There is a dual percolation cluster pictured in thick grey solid lines.

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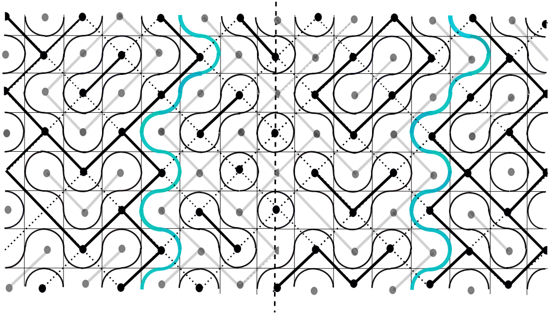

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Result. Loop (cluster) density for odd $L = 2N + 1$.

(A.P., A. Trofimova ,2024)

- Exact formula:

$$\nu(2N+1) = \frac{1}{1+2N}\left(\frac{\Gamma(\frac{N}{2})\Gamma(\frac{3}{2}+\frac{3N}{2})}{\Gamma(\frac{3N}{2})\Gamma(\frac{1}{2}+\frac{N}{2})} + \frac{\Gamma(\frac{1}{2}+\frac{N}{2})\Gamma(2+\frac{3N}{2})}{\Gamma(1+\frac{N}{2})\Gamma(\frac{1}{2}+\frac{3N}{2})}\right) - \frac{5}{2}$$
$$= \frac{1}{12}, \frac{37}{400}, \frac{597}{6272}, \frac{2441}{25344}, \frac{78035}{805376}, \ldots,$$

- Asymptotic expansion:

$$\nu(L) = \frac{3\sqrt{3}-5}{2} - \frac{1}{4\sqrt{3}}L^{-2} + \frac{35}{144\sqrt{3}}L^{-4} + O(L^{-6}).$$

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O(1) DLM/percolation on tilted lattice

How does the change of the lattice orientation affects the loop/cluster densities?

O(1) DLM/percolation on tilted lattice

- Fix two non-negative co-prime integers $m, n \in \mathbb{N}_0$, which are not zero simultaneously, and positive integer $l \in \mathbb{N}$, such that

$$L = (m+n)l \in 2\mathbb{N}$$

  is an even positive integer.

- Consider O(1) DLM on a strip of the square lattice $\mathscr{L} = (V, E)$ with $V = \{1, \ldots, ln\} \times \mathbb{Z}$ and $E = \{(v, v+\boldsymbol{e}_x), (v, v+\boldsymbol{e}_y))\}_{v \in V}$, rolled into a cylinder with helical boundary conditions, i.e. $v \equiv v + nl \cdot \boldsymbol{e}_x - ml \cdot \boldsymbol{e}_y$ for any $v \in V$ introducing a tilt with angle α, such that $\tan\alpha = m/n$.

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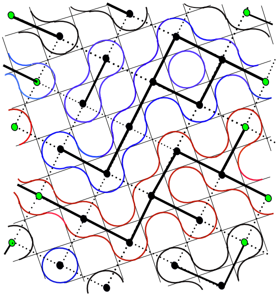
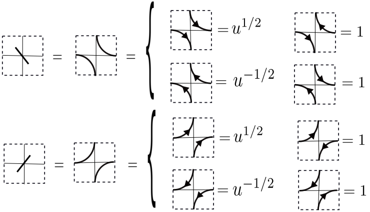


Inhomogeneous six vertex model (Fujimoto, 1994)

Auxiliary vertices.



Tilted lattice from in-homogeneous model.

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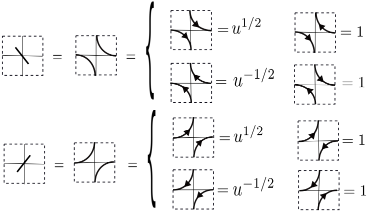

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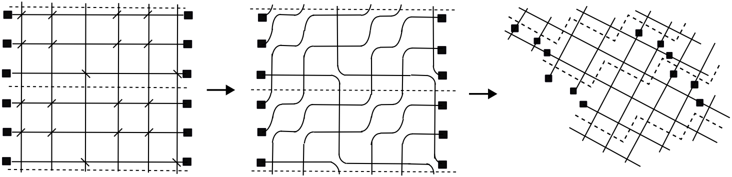

Results. Loop/cluster densities. $m = n = 1$ (A.P. 2023)

l	$\nu_{\mathrm{c}}(l,1,1)$	$\nu_{\mathrm{nc}}(l,1,1)$	$\nu(l,1,1)$
1	$\frac{1}{6}$	$\frac{1}{3}$	$\frac{1}{2}$
2	$\frac{13}{110}$	$\frac{9}{110}$	$\frac{1}{5}$
3	$\frac{1423}{13338}$	$\frac{229}{6669}$	$\frac{11}{78}$
4	$\frac{1113499}{10834754}$	$\frac{405855}{21669508}$	$\frac{677}{5572}$
5	$\frac{5979030577}{59179172262}$	$\frac{1747404017}{147947930655}$	$\frac{85013}{753370}$
6	$\frac{217910906936461}{2176660978677230}$	$\frac{17718816661443}{2176660978677230}$	$\frac{1996408}{18442085}$
7	$\frac{119374505844765596 3}{1198955429720436937 8}$	$\frac{24990014509495090 7}{41963440040215292823}$	$\frac{3347923855}{31727676806}$
8	$\frac{883507164842364573251 9}{890513512484922349136 74}$	$\frac{161979677703475304863 5}{356205404993968939654696}$	$\frac{208657158071}{2010948047656}$
9	$\frac{3973328570636277936805618733}{40145601162806730995798838798}$	$\frac{7199386081737931240669171 7}{200728005814033654978994193 99}$	$\frac{77376513420899}{754454218879206}$

Table: Exact densities of critical percolation clusters on the lattice in standard orientation rolled into a cylinder, $n = m = 1$.

Results. Loop/cluster densities. $m = 3, n = 4$ (A.P. 2023)

l	$\nu_{\mathrm{c}}(l,3,4)$
2	$\frac{387768065791915313}{389595385018232242 6}$
4	$\frac{4419511640697444058108156606728951059893148419416069897893461373881296882006 5999}{4489650927690021586742048185446868461439859589378842558689286573006104887469 52074}$

l	$\nu_{\mathrm{nc}}(l,3,4)$
2	$\frac{113439513997319 31}{194797692509116121 3}$
4	$\frac{3247033799919876057720749558083030828173963225205778321555204455812502140070 26}{2244825463845010793371024092723434230719929794689421279344643286503052443734 76037}$

l	$\nu(l,3,4)$
2	$\frac{505753025}{4800491638}$
4	$\frac{1025205092866657199069018079406719010967}{1026393564075777521889005568904945162265 8}$

Finite size corrections. Numerical check. **(A.P. 2023)**

- The universal CFT based $O(l^{-2})$ finite size correction is expected to depend on n and m only via the length rescaling $l \to \tilde{l} = l\sqrt{(m^2+n^2)/2}$, while the coefficients of the next corrections be the periodic functions of quadruple the tilt angle $\alpha = \arctan(m/n)$.

$$\nu(l,n,m) = \nu(\infty,n,m) + \frac{5\sqrt{3}}{24}\frac{1}{\tilde{l}^2} + \frac{a(\alpha)}{\tilde{l}^4} + \frac{b(\alpha)}{\tilde{l}^6}$$

- $$\begin{aligned} a(\alpha) &\simeq -0.0125 - 0.192\cos(4\alpha) \\ b(\alpha) &\simeq 0.00760 + 0.0273\cos(4\alpha) + 0.495\cos(8\alpha) \end{aligned}$$

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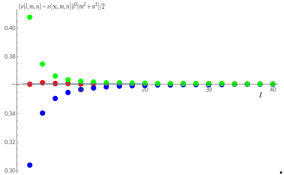

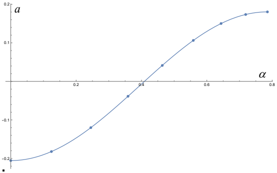

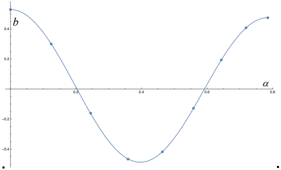

Conclusion and Perspectives

Done:

- We obtained the closed formulas for exact densities of loops and critical percolation clusters on a cylinder of standard orientation (even and odd circumference)
- We developed the procedure of calculating densities for tilted lattices wrapped to cylinders of finite circumference. Numerics based conjectures are proposed for the dependence of finite size corrections on the tilt.

To be done:

- Loops and percolation with various boundary conditions and on different lattices
- Higher cumulants
- More general correlation functions.

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References

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THANK YOU!