The Shape of Ice

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The Ice model

Let **G** be a connected graph without self loops and with even vertex degree. Orient each edge of **G** in the following way.

Definition

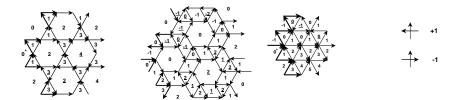
A **vertex configuration** is the arrangement of arrows arriving to and departing from a vertex. It is **legal** for the **lce rule** if there is the same number of incoming and outgoing arrows. If there is a legal vertex configuration at every vertex of **G** the arrow configuration is legal for the **lce model**.

On ${\bf G}={\bf Z}^2$ Ice is also known as the **Six vertex model**. It is a remarkably good model for the physical ice. Analyzed by E. Lieb et. al. in the 60's.

Until recent years little was known about this model in a bounded domain.

Lattices

Archimedean/uniform lattices are the natural generalizations of the three regular lattices. They are formed as vertex and edge sets of the tilings of the plane by convex regular polygons. Of the 11 Archimedean lattices four support Ice: **square, triangular, Kagomé and 3.4.6.4. lattices** (6/20/18/36 vertex rules respectively).



Kagomé (K), 3.4.6.4. and triangular (T) lattices with height on the dual.

Bounded case: known unknowns

For simplicity we consider here these models in particular domains: the square lattice lce in a **diamond/square**, the others in a **hexagon** (with sides aligned with the lattice lines).

Questions:

- When is a boundary arrangement of arrows legal i.e. allowing a fill-in? When does it allow multiple fill-ins? Exponential number of fill-ins?
- In case of multiple fill-ins, is there long range boundary influence? If so, what is the structure inside generically like? These are questions about the support of the measure of maximal entropy.
- Are the four vertex models behaving alike i.e. is there universality?

The investigation was initially motivated by the **Dimer/Domino model** studies by Propp et. al. related to crystal growth, faceting etc.

Cycles

A basic observation: in an Ice configuration an unidirectional cycle can be reversed (infinite cycle, too, if existing).

Definition

Depending on the lattice 1-triangle/1-square/1-lozenge/1-hexagon denotes the smallest such polygon. If such 1-polygon is unidirectional we call it a 1-cycle and the reversal of this orientation a local move/flip.

Later we will also need to keep track of the geometric orientation of the triangles and lozenges, but let's keep it simple now.

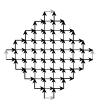
Proposition

An unidirectional cycle always encloses a 1-cycle.

Proof is a simple argument utilizing the flux across the cycle.

Boundary cosets

A cycle is **off-boundary** if it doesn't contain any of the boundary arrows. A configuration is **frozen** if it is without off-boundary 1-cycles. A **temperate** configuration has a directed cycle boundary.





Basic question: Given a fixed boundary, a frozen configuration cannot be deformed but what about the others?

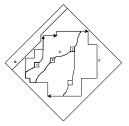
Connectivity

Theorem

The set of Ice configurations with common boundary arrows in a diamond (for square lattice) and in a hexagon (the other three Archimedean lattices) is connected under 1-cycle reversals i.e. two such configurations can be transformed to each other with a finite sequence of 1-cycle reversals.

Two lines of proof:

- 1. **lexicographic sweep** removes the difference between two configurations with identical boundaries site by site from the boundary on.
- 2. **height argument** converts each local height minimum to a maximum eventually connecting the configurations via a maximal configuration, all with the given boundary configuration.



Connectivity, computation

Through counterexamples one sharpens this to

Upgrade

If for triangular/Kagomé/3.4.6.4 lattice any one of the 2/3/6 types of local moves is disallowed the previous Theorem fails.

Ice through dynamics:

- 1. Divide the arrow configurations into arrays of oriented 1-polygons:
 - Z²: checkerboard: black and white/even and odd arrays of 1-squares.
 - **T**: two arrays of 1-triangles (\triangle and ∇).
 - K: two 1-triangle and one 1-hexagon arrays.
 - 3.4.6.4: two 1-triangle, one 1-hexagon and three 1-lozenge arrays (right & left-leaning and straight standing).

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Probabilistic cellular automata

2. In an array flip the orientation of each off-boundary 1-cycle independently w.p. 1/2 and update the other arrays. This gives a random map F_{array} on the configurations with a given boundary. Independent sequences of F-maps define the PCAs:

- \mathbf{Z}^2 : { F_e , F_o }.
- T: $\{F_{\triangle}, F_{\bigtriangledown}\}$.
- ullet K: $\{ \emph{F}_{\triangle}, \emph{F}_{igtriangle}, \emph{F}_{hex} \}$.
- $\bullet \ \ \textbf{3.4.6.4:} \ \{ \textit{F}_{\triangle}, \textit{F}_{\bigtriangledown}, \textit{F}_{\textit{hex}}, \textit{F}_{\textit{I}-\diamondsuit}, \textit{F}_{\textit{r}-\diamondsuit}, \textit{F}_{\textit{s}-\diamondsuit} \} \, .$

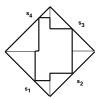
These PCAs, **the Dynamic Ice models**, are irreducible and aperiodic Markov Chains hence **ergodic**. In all our runs they relaxed to the equilibrium i.e. to the measures of maximal entropy at an exponential rate.

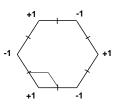
Frozen areas

If the boundary configuration is such that the flux into the domain is zero then there is a fill-in.

Call the discrete derivative of the height along a contiguous boundary segment the **tilt** of the segment. A boundary segment of maximal tilt ± 1 uniquely determines the configuration in an interior wedge.







Max tilt for **Z**², wedges in a diamond and a frozen corner lozenge for **T/K**.

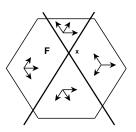
Entropy

The **entropy of a boundary condition** for a diamond/hexagon denotes the exponential size of the set of its legal fill-inns: $h_N = \frac{\log(\# \text{ of configurations})}{\# \text{ of arrows}}$, where # denotes the number on the entire domain.

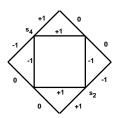
Proposition

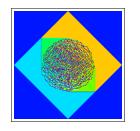
On the square, triangular and Kagomé lattices the entropy can attain arbitrarily small positive values in the scaling limit.

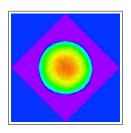
For K, T consider the seed configuration on the right. Subdomain F will remain frozen for all times and the rest will have positive density of say even unidirectional 1-triangles. Moving x towards the rightmost corner gives an arbitrary low positive upper bound for the entropy. Analogous argument on Z^2 .



Arctic geometry in a **Z**² diamond





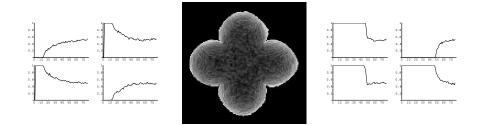


Ridge roof boundary, vertex configuration and cumulative flip count. Inscribed square has Korepin's DWBC.

102-diamond, equilibrium snapshot at 20.000 (rendered from 1-square array), followed by 5.000 iterate flip collection (from [E1], -99)



Z² sectional probabilities



Center: Inverted flip density in the clover (diamond rotated by 45 degrees). Left and Right: Horizontal and diagonal sections of orientation probabilities for the arrows.

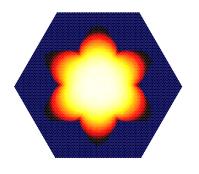
75-diamond, 2500 iterates at the equilibrium.

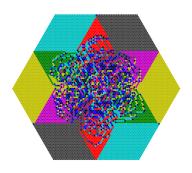


Arctic geometry of spatial phase transition

- In the scaling limit (lattice spacing → 0 in a unit polygon) boundaries with extremal tilt segments can imply spatial phase transition curves in the interior separating frozen and temperate domains. The Arctic Circle first established by Jockush, Propp and Shor for dominoes in Aztec diamond. A variational principle proof for the Z² dominoes/dimers by Cohn, Kenyon and Propp, later generalized to bipartite graphs by Kenyon, Okounkov and Sheffield. The domain shape need not to be finely tuned.
- At the free fermion point the domino results carry over to Ice on the square lattice. The bulk properties depend on the boundary. In square Ice the Arctic Curve Phenomenon seems to extend well in to the disordered regime ($-1 < \Delta < 1$) and to other lattices as well. In particular the **triangular and Kagomé lattice Ice models exhibit clear Arctic Curve behavior**. No universality though.

Arctic geometry on T/K

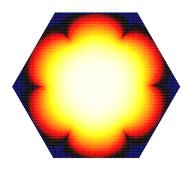


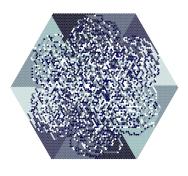


Cumulative flip count and vertex configuration snapshot at equilibrium on T.

99-hexagon, 10^5+10^5 iterates at equilibrium, boundary cond. as before. ([E2], -13)

Arctic geometry on **T**/**K**







Boundary tilts, cumulative flip count and filtered configuration at equilibrium on ${\bf T}$.

99-hexagon, $10^5 + 2 \cdot 10^5$ iterates.

Extremal tilt on 3.4.6.4.

From the periodicity properties of 3.4.6.4. lattice one can derive

Proposition

Consider a 3.4.6.4. configuration on a hexagon and a n-block of consecutive boundary arrows along any of its straight edges. If the boundary arrows are of period eight in such a block the height over the block satisfies $|\Delta h| \leq (3n+7)/4$. For an arbitrary n-block of arrows, $n \geq 15$, the bound is $|\Delta h| \leq (13n+28)/15$. Hence if the boundary height exists in the scaling limit and has tilt, the absolute value of the latter cannot exceed 13/15.

Hence there are no boundary assignments of arrows with extremal tilt ± 1 .

Entropy

Proposition

In any 3.4.6.4. Ice configuration in the set of 1-triangles and 1-lozenges at least 1/7 of them are unidirectional. If the scaling limit entropy for a given boundary exist, it is bounded from below by $\frac{1}{24} \log 2$.







Finding any low entropy boundary is hard: $\frac{1}{6} \log 2$ can be attained, seeded by the hexagon.

No-go

To summarize:

Theorem

There are no frozen configurations in 3.4.6.4. Ice. No frozen/temperate spatial phase transition in the scaling limit and no corresponding Arctic curve. The low entropy result of the three other Archimedean Ice models fails for 3.4.6.4. No Archimedean universality.

For all 3.4.6.4. boundary conditions checked the equilibrium configurations appeared rather homogeneous. Gas/liquid boundary not excluded though.

Rest

[E1] Diamond Ice, *J. of Stat. Phys.* $\bf 96$, 5/6, pp. 1091-1109, 1999, math.aalto.fi/ \sim kve/research.html.en

[E2] Archimedean Ice, Discr. and Cont. Dynamical Systems 33, 9, 2013, arXiv:math-ph/0909.4007

Thank you

Robert Mangold, 1972 RISD museum. Providence