Large deviations for the 3D dimer model

Catherine Wolfram
(joint work with Nishant Chandgotia and Scott Sheffield)
July 13, 2023

Massachusetts Institute of Technology

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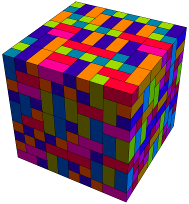

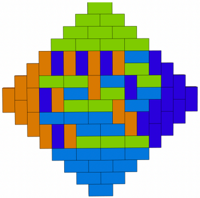

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Introduction

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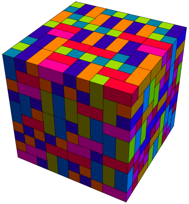
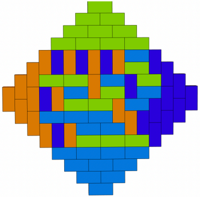




The main goal is to explain how to generalize the large deviation principle for dimer tilings in $\mathbb{Z}^2$ by Cohn, Kenyon, and Propp [1].

There are two main challenges that make studying dimers in 3D different from 2D:

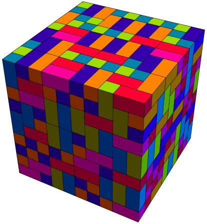
- There is no height function correspondence for dimer tilings of $\mathbb{Z}^3$.
- There are no (known) formulas for the partition function, surface tension, etc for tilings of $\mathbb{Z}^3$. (And the model is probably not integrable.)

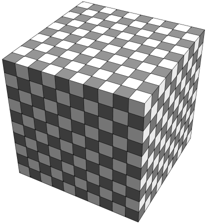
Plan for the talk

- A bit more about these two ways that studying the dimer model in 3D is different from 2D
- Set up for an LDP and analogous result in 2D
- Main theorems in 3D
- Simulations!
- A few methods that we use in the proofs in 3D.

Correspondence: dimer tilings and discrete vector fields

For any d, $\mathbb{Z}^d$ is a bipartite lattice, with underlying black and white checkerboard.





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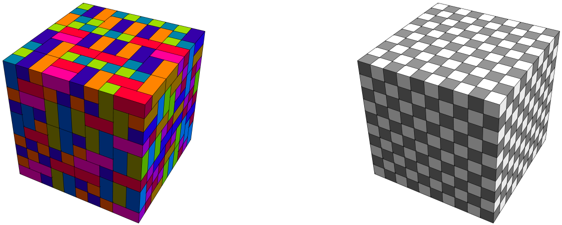

The colors of the dimers represent the cardinal direction of the dimer (north, south, east, west, up, down for $d = 3$), viewed as a vector from its white cube to its black cube.

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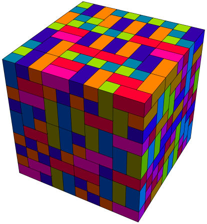

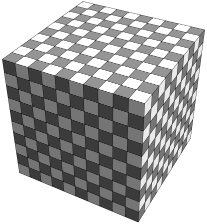

The colors of the dimers represent the cardinal direction of the dimer (north, south, east, west, up, down for $d = 3$), viewed as a vector from its white cube to its black cube.

There is a correspondence between 1) a dimer tiling τ of $\mathbb{Z}^d$ and 2) a *discrete vector field* v_τ defined by: for each edge e of $\mathbb{Z}^d$ oriented from white to black,

$$v_\tau(e) = \begin{cases} 1 & e \in \tau \\ 0 & e \notin \tau \end{cases}$$

Height function replacement: divergence free discrete vector field

Observation: compute divergences of v_τ.

$$\operatorname{div} v_\tau(x) = \sum_{\substack{e \ni x \\ \text{oriented out of } x}} v_\tau(e) = \begin{cases} +1 & x \text{ is white} \\ -1 & x \text{ is black.} \end{cases}$$

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Subtracting a constant reference flow $r(e) = 1/(2d)$ for all $e \in \mathbb{Z}^d$, a dimer tiling τ corresponds to a divergence free discrete vector field f_τ which we call the ***tiling flow***.

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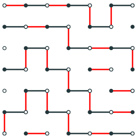
The main intuition throughout this talk is to think of a dimer tiling as a *flow*.

Remark: non-intersecting paths and (non)-integrability?

One of the ways to see that the dimer model on $\mathbb{Z}^2$ is integrable is via the bijection with *non-intersecting paths* in $\mathbb{Z}^2$ by overlaying a tiling (red) with a brickwork tiling (black).



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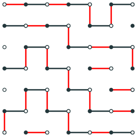
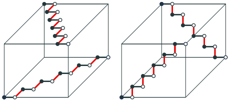


There is an analogous bijection between dimer tilings of $\mathbb{Z}^3$ and non-intersecting paths in $\mathbb{Z}^3$. But these paths are not ordered, they can be braided in various ways, etc.



Part II: set up for an LDP and 2D context

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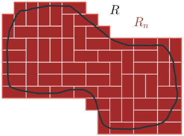

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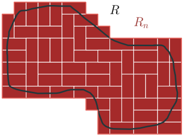

Question: what do uniform random dimer tilings of R_n look like in the fine-mesh limit as $n \to \infty$?

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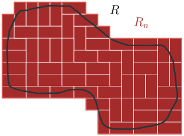

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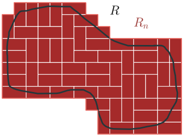

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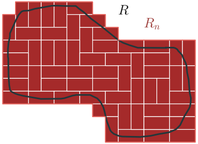
Large deviations means quantifying: given a deterministic flow g, what is the probability that a tiling of R_n is close to g as $n \to \infty$? There is a *limit shape* if is there is one flow that random tilings concentrate on as $n \to \infty$.

Ingredients of an LDP



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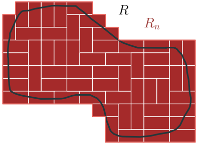

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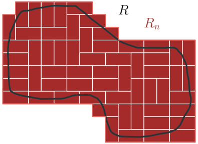

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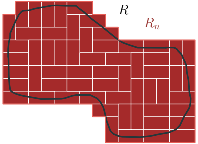

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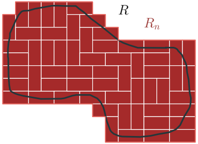

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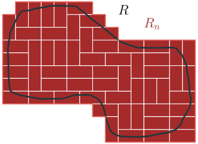

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5. Main step for proving that $I(\cdot)$ has a unique minimizer is usually to prove that $I(\cdot)$ is *strictly convex*.

Fix $R \subset \mathbb{R}^2$ compact simply connected region, h_b boundary height function. Choose $R_n \subset \frac{1}{n}\mathbb{Z}^2$ regions approximating R such that boundary values of height functions for tilings of R_n converge to h_b.

Context: LDP and limit shape theorems in 2D by Cohn, Kenyon and Propp

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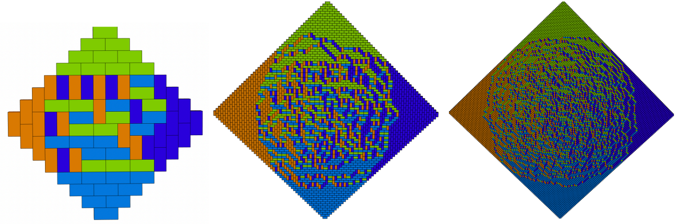

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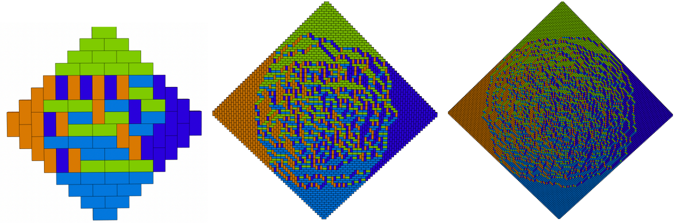

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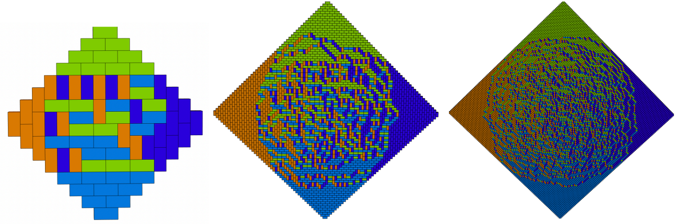

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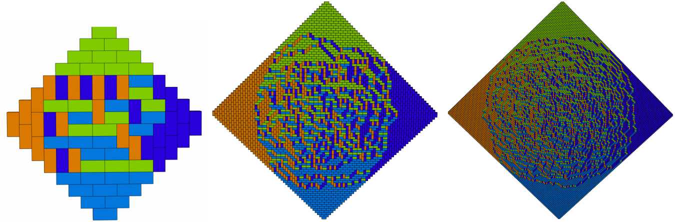

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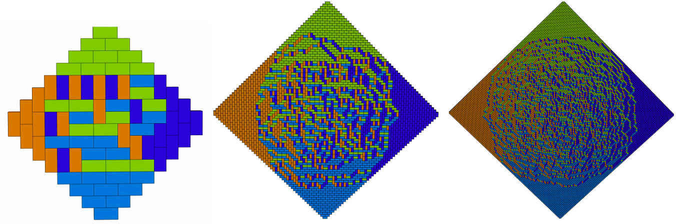

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- **Rate function**: $I : AH(R, h_b) \to [0, \infty)$ has the form

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The entropy function $\text{ent}_2 : \{(s,t) : |s| + |t| \leq 2\} \to [0, \infty)$ can be **computed explicitly** using Kasteleyn theory (linear algebra), and this is the main tool in 2D for showing strict convexity and proving that I has a unique minimizer with each boundary condition h_b.

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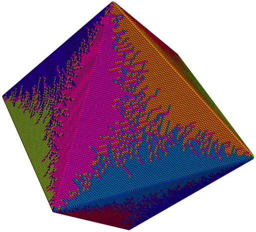
The formula is

$$\text{ent}_2(s_1, s_2) = \sum_{i=1}^{4} L(\pi p_i),$$

where p_i are determined by (s_1, s_2) with the equations $p_1 + p_2 + p_3 + p_4 = 1$, $s_1 = 2(p_1 - p_2), s_2 = 2(p_3 - p_4)$, and $\sin(\pi p_1)\sin(\pi p_2) = \sin(\pi p_3)\sin(\pi p_4)$ and $L(z) = \int_0^z \log|2\sin t|\,\mathrm{d}t$ is the *Lobachevsky function.*

Part III: moving to three dimensions



Need to explain:

- Measures ρ_n;
- Topology for comparing tilings, and corresponding fine-mesh limits [different from 2D since we don't have a height function]
- Rate function I [methods to understand this are different from 2D because we do not have a formula for it]

Will explain the first two, then state the main theorems in 3D. After that, will describe the rate function. (Then show simulations, and say a little bit about our methods.)

Topology in 3D: use tiling flows

Recall that any dimension d, there is a correspondence

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Topology: induced by a metric d_W on tiling flows, where d_W is a version of *Wasserstein distance*.

Topology in 3D: use tiling flows

Recall that any dimension d, there is a correspondence

$$\left\{\text{dimer tilings } \tau \text{ of } \mathbb{Z}^d\right\} \qquad \Longleftrightarrow \qquad \left\{\text{div free discrete flows } f_\tau\right\}.$$

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Intuitive description of d_W: two flows are close if we can transform one flow into another with low "cost" where "cost" is the minimum sum of 1) amount of flow moved times distance moved, 2) flow added, 3) flow deleted to transform one flow into the other.

The fine-mesh limits as $n \to \infty$ of tiling flows in this topology are *asymptotic flows*, which are vector fields on R that are

- measurable
- divergence-free (as a distribution)
- valued in the *mean-current octahedron*

$$\mathcal{O} = \{s = (s_1, s_2, s_3) : |s_1| + |s_2| + |s_3| \leq 1\}.$$

A element $s \in \mathcal{O}$ is called a *mean current*.

Measures ρ_n: hard and soft boundary conditions

Fix a nice region $R \subset \mathbb{R}^3$ (compact, closure of a domain, ∂R piecewise smooth) and b a boundary value on ∂R.

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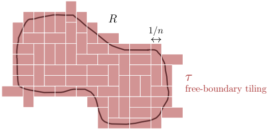

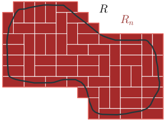

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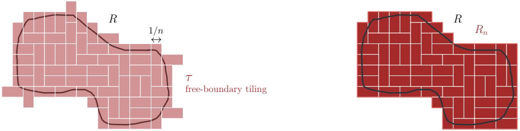

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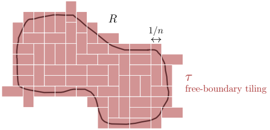

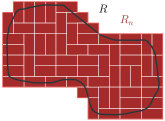

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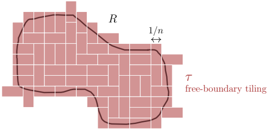

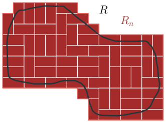

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Soft boundary (SB): choose a sequence of “thresholds” $(\theta_n)_{n \geq 0}$ with $\theta_n \to 0$ slowly enough and let ρ_n be uniform measure on free-boundary tilings of $R \cap \frac{1}{n}\mathbb{Z}^3$ with boundary values within θ_n of b.

Main theorems in 3D summarized

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(R, b)	SB LDP (ρ_n)	Ent maximizer/I_b minimizer unique	HB LDP $(\overline{\rho}_n)$
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For (R, b) rigid, a *weak uniqueness* holds. Namely, if f_1, f_2 are both Ent maximizers, then on the set A where they differ they are both valued in $\mathcal{E}$.

For either $(\rho_n)_{n\geq 1}$ (soft boundary) or $(\overline{\rho}_n)_{n\geq 1}$ (hard boundary), the *rate function* when an LDP holds is

$$I_b(g) = C - \mathrm{Ent}_3(g).$$

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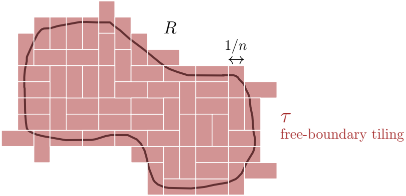
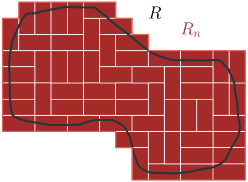
Here $h(\mu)$ is specific entropy (limit of Shannon entropy per site) and $\mathcal{P}^s$ is "measures with mean current s", i.e. the set of measures on dimer tilings of $\mathbb{Z}^3$ which are invariant under even translations (these are the translations that preserve the direction of flow) such that the μ-expected flow through the origin is $s \in \mathcal{O}$.

Dictionary between 2D LDP and 3D LDP set ups

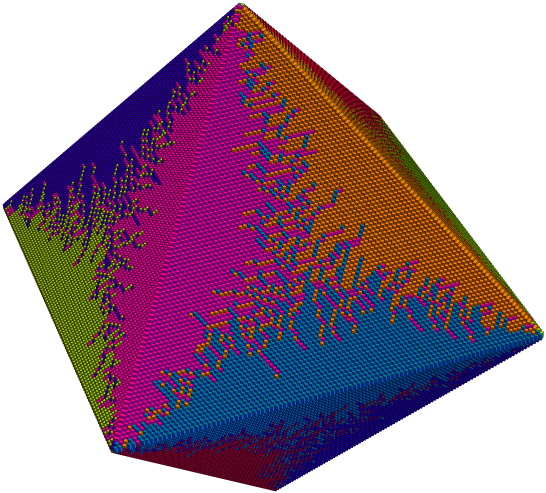
	2D	3D
compact region R that is...	simply connected [1], multiply connected [3]	closure of connected domain, ∂R piecewise smooth
object associated to tiling τ	height function h	tiling flow f_τ
topology (to compare tilings)	sup norm on height functions	Wasserstein metric d_W on tiling flows
limits of discrete objects	asymptotic height functions: 2-Lipschitz functions	asymptotic flows: div-free meas. vector fields valued in $\mathcal{O}$
rate function	$C_2 - \mathrm{Ent}_2(\nabla h)$	$C_3 - \mathrm{Ent}_3(f_\tau)$





Part IV: simulations

Simulations: aztechedron and slices



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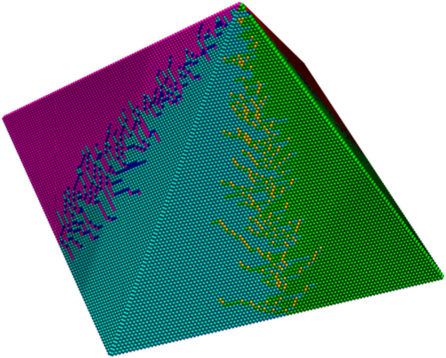

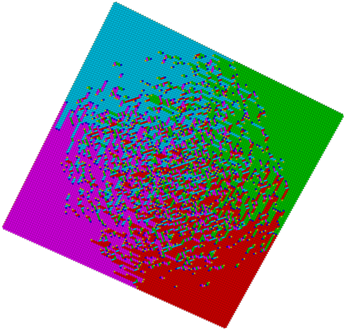

Part V: a few methods

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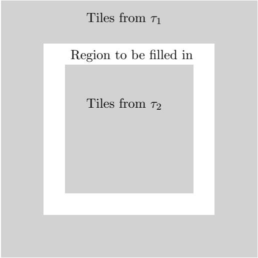

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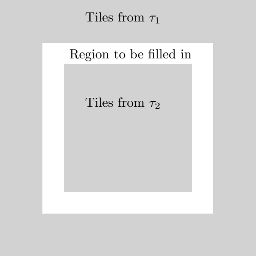

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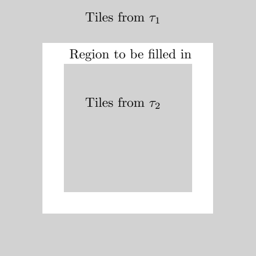

- In 2D, patching is proved using Lipschitz extension theorems for height functions. Our arguments in 3D are very different and more combinatorial.
- **strict convexity** of the rate function I_b (more precisely, strict concavity of ent) and how to understand I_b without formulas.

Patching: more precisely

Let $B_n = [-n, n]^3$ and fix $\delta > 0$. If two tilings τ_1, τ_2 of $\mathbb{Z}^3$ approximate the constant flow $s \in \mathrm{Int}(\mathcal{O})$, how can we show that we can "patch them together" with τ_1 outside B_n to τ_2 inside $B_{(1-\delta)n}$ by tiling the annulus $A_n = B_n \setminus B_{(1-\delta)n}$ between them?

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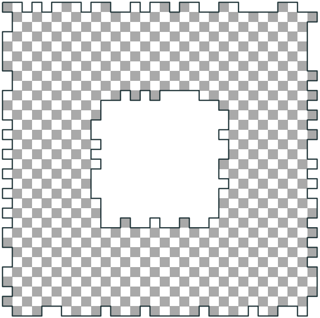

In other words, under what conditions is an annular region like the one above exactly tileable by dimers?

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Hall’s matching theorem [2] gives a necessary and sufficient condition:

Theorem. A balanced region $R \subset \mathbb{Z}^3$ is tileable by dimers if and only if there is no *counterexample set* $U \subset R$, i.e. no set of cubes which has $\text{white}(U) > \text{black}(U)$, despite having only black cubes along its boundary within R.

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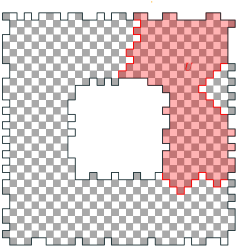

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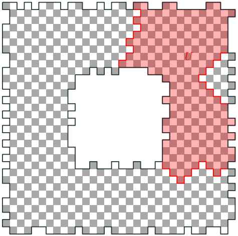

To prove the patching theorem, we show that there are no counterexamples to tileability of A_n when n is large enough and apply Hall's matching theorem.

Unlike in 2D, we do **not** have a formula for ent(s) in Int($\mathcal{O}$).

Understanding the rate function I_b

Unlike in 2D, we do **not** have a formula for $\mathrm{ent}(s)$ in $\mathrm{Int}(\mathcal{O})$.

To prove that the rate function

$$I_b(g) = C - \mathrm{Ent}(g) = C - \frac{1}{\mathrm{Vol}(R)} \int_R \mathrm{ent}(g(x))\,\mathrm{d}x$$

has a unique minimizer, one of the important steps is to show that $\mathrm{ent}(s)$ is *strictly concave* on $\mathcal{O} \setminus \mathcal{E}$, where $\mathcal{E}$ is the edges of $\mathcal{O}$.

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Without a formula for ent we need "soft arguments" for strict concavity. The main idea, for $s \in \mathrm{Int}(\mathcal{O})$, is a method called *chain swapping*.

Before explaining chain swapping, want to explain some background about *Gibbs measures*.

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- **Corollary of the patching theorem**: if μ_1, μ_2 are *ergodic Gibbs measures* (EGMs) of the same mean current $s \in \mathrm{Int}(\mathcal{O})$, then $h(\mu_1) = h(\mu_2)$.

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- **Corollary of the patching theorem**: if μ_1, μ_2 are *ergodic Gibbs measures* (EGMs) of the same mean current $s \in \mathrm{Int}(\mathcal{O})$, then $h(\mu_1) = h(\mu_2)$.

Idea with chain swapping: uses two measures μ_1, μ_2 of mean currents s_1, s_2 to construct new two measures with mean currents $(s_1 + s_2)/2$ and the same total entropy, but then show that this breaks the Gibbs property.

Chain swapping and $\mathrm{ent}(s)$ for $s \in \mathrm{Int}(\mathcal{O})$

Let $\mu = (\mu_1, \mu_2)$ be a measure on pairs of dimer tilings which is invariant under even translations, sample (τ_1, τ_2) from μ. The union $\tau_1 \cup \tau_2$ is a collection of double tiles, finite loops, and *infinite paths*.

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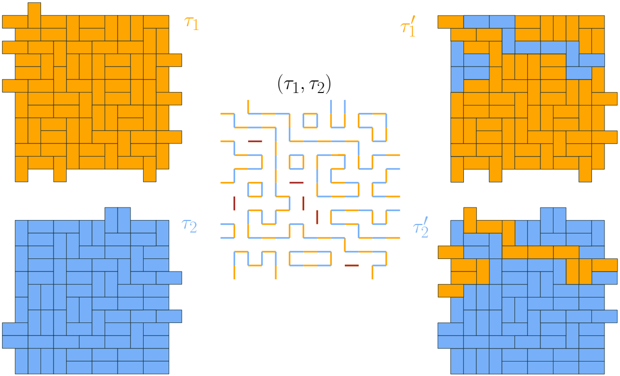

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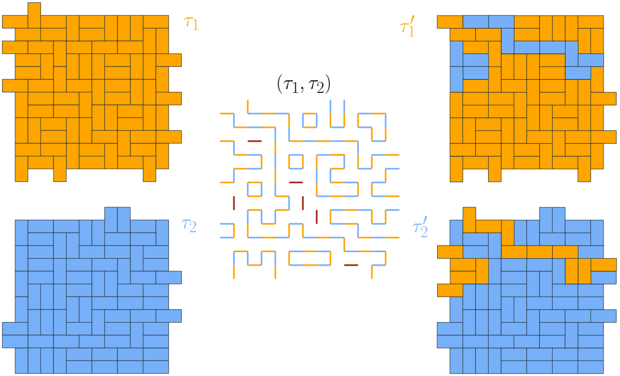

Chain swapping: for each infinite path "of nonzero slope" $\ell \subset (\tau_1, \tau_2)$, with independent probability 1/2 we swap the tiles from τ_1, τ_2 to construct a new pair of tilings (τ_1', τ_2'). This defines a new *swapped measure* $\mu' = (\mu_1', \mu_2')$.

Suppose μ is an erogdic coupling of ergodic measures μ_1, μ_2 on dimer tilings, with mean currents $s(\mu_1) \neq s(\mu_2)$. Let μ' be the swapped measure, with marginals μ_1', μ_2'. Chain swapping...

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Chain swapping to prove strict concavity on $\mathrm{Int}(\mathcal{O})$

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Chain swapping to prove strict concavity on Int($\mathcal{O}$)

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proof* of strict concavity for $s \in \mathrm{Int}(\mathcal{O})$: Given mean currents $s_1 \neq s_2$, $\frac{s_1+s_2}{2} \in \mathrm{Int}(\mathcal{O})$, let μ_1, μ_2 Gibbs be such that $\mathrm{ent}(s_i) = h(\mu_i)$. Assuming that μ_1, μ_2 are EGMs*, then by chain swapping

$$2\mathrm{ent}\left(\frac{s_1 + s_2}{2}\right) > h(\mu_1') + h(\mu_2') = h(\mu_1) + h(\mu_2) = \mathrm{ent}(s_1) + \mathrm{ent}(s_2).$$

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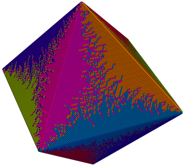
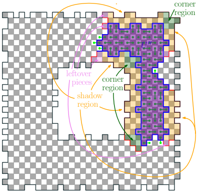
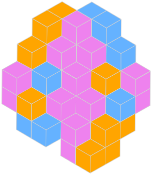
*full proof uses case work based on ergodic decompositions (we don't yet know that EGMs of every mean current exist) but this is the main idea.

Thank you for listening!!







Various open questions...

- Is there is a unique EGM of mean current s for all $s \in \mathrm{Int}(\mathcal{O})$?
- What can be said about the interfaces between frozen and liquid regions in the limit shapes? How big should the fluctuations be?
- Do there exist regions $R \subset \mathbb{R}^3$ (with ∂R piecewise smooth) and boundary conditions b where (R, b) has more than one Ent maximizer?
- Now we know a limit shape *exists*. Are there soft arguments, for example, for the existence of frozen regions in the limit shape?
- and more...