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Six-vertex model and Schramm-Loewner evolution

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Square ice is a statistical mechanics model for two-dimensional ice, widely believed to have a conformally invariant scaling limit. We associate a Peano (space-filling) curve to a square ice configuration, and argue that its scaling limit is a space-filling version of the random fractal curve SLEκ, Schramm-Loewner evolution with parameter κ, where \(4 < \kappa \leq 12 + 8\sqrt{2}\). For square ice, \(\kappa = 12\). At the “free-fermion point” of the six-vertex model, \(\kappa = 8 + 4\sqrt{3}\). These unusual values lie outside the classical interval \(2 \leq \kappa \leq 8\).

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I. INTRODUCTION

Square ice was introduced by Pauling [1] as a model of hydrogen bonding in ice crystals in two dimensions [2]. A square-ice configuration is an orientation of each edge of the square lattice, subject to the constraint that each vertex has two incoming and two outgoing edges (see the diagram below and Fig. 1). Recently actual square ice crystals were produced between sheets of graphite [3].

The classical six-vertex model from statistical mechanics generalizes square ice by adding energies to each of the six types of local configuration at a vertex:

\[
\begin{array}{cccccc}
\varepsilon_1 & \varepsilon_2 & \varepsilon_3 & \varepsilon_4 & \varepsilon_5 & \varepsilon_6
\end{array}
\]

Square ice is the uniform measure on six-vertex configurations. The six-vertex model partition function was famously solved by Lieb in 1967 [4]. A number of beautiful combinatorial identities arising in this model have intrigued mathematicians and physicists for many years [5,6]. In particular it is widely believed that the six-vertex model has conformally invariant scaling limits; however, a mathematical proof of this fact is lacking.

We show here how to associate a discrete Peano (space filling) curve to configurations of the square ice model with appropriate boundary conditions (Fig. 1). We present evidence that the scaling limit of this curve is a random fractal curve called a Schramm-Loewner evolution (SLE).

For each \(\kappa \leq 0\), an SLEκ in the upper half plane is a random non-self-crossing random curve that extends from the origin to \(\infty\), with the parameter \(\kappa\) indicating how “windy” the path is. In recent decades, SLE has been thoroughly studied and celebrated within both physics and mathematics and has led to many new results about two-dimensional statistical physics and the Liouville theory of quantum gravity, some of which go far beyond the results previously established using conformal field theory and other techniques.

The precise definition of SLE is interesting and indirect. Fix \(\kappa > 0\), let \(B_t\) be a one-dimensional Brownian motion, and for each \(z\) in the complex upper half plane \(\mathbb{H}\), let \(g_t(z)\) solve the ODE

\[
\frac{\partial g_t(z)}{\partial t} = \frac{2}{g_t(z) - \sqrt{\kappa} B(t)} - \frac{\partial g_0(z)}{\partial t} = z,
\]

which is defined until \(T_z = \inf\{t : g_t(z) - W_t = 0\}\). Then SLEκ is the curve \(\eta : \mathbb{R}_+ \to \mathbb{H}\) defined so that \(\{z : T_z \leq t\}\) is the set of points hit or cut off from \(\infty\) by \(\eta([0,t])\).

For \(\kappa \leq 4\), SLEκ is a simple curve; for \(4 < \kappa < 8\), the curve hits itself without crossing itself, forming bubbles; for \(\kappa \geq 8\), the curve is space-filling [7]. For \(4 < \kappa < 8\), there is also a space-filling version of SLEκ in which the bubbles get filled in recursively as they are made [8].

The SLEκ curves are either known or believed to characterize the scaling limits of various two-dimensional critical statistical physics models: dilute polymers (\(\kappa = 8/3\)) [9], dense polymers (\(\kappa = 8\)) [10], loop-erased random walk (\(\kappa = 2\)) [10], percolation interfaces (\(\kappa = 6\)) [11], Ising model spin clusters (\(\kappa = 3\)) [12,13], dimer systems (\(\kappa = 4\)), contours of the Gaussian free field (\(\kappa = 4\)) [14,15], the Ashkin–Teller model (\(\kappa = 4\)), the Fortuin–Kasteleyn random cluster model (\(2 \leq \kappa \leq 8\)), active spanning trees (\(4 < \kappa \leq 12\)) [16], and others. The dimension \(D_f\) of the fractal increases with the parameter \(\kappa\) according to the formula \(D_f = \min\{2,1 + \kappa/8\}\) [7,17]. See Refs. [7,18,19] for further background.

SLE is connected with conformal field theory (CFT) [18], where the central charge \(c\) is related to \(\kappa\) by

\[
c = (8 - 3\kappa)(\kappa - 6)/2\kappa.
\]

In CFT usually \(c \geq -2\), which corresponds to \(\kappa \in [2,8]\), the values relevant to conformal loop ensembles [20]. Before this work and Ref. [16] it was widely assumed that only \(\kappa \in [2,8]\) would appear in natural discrete models [18].

For the six-vertex model Peano curve defined here, \(\kappa\) depends on the vertex energies and spans the range \((4,12 + 8\sqrt{2})\), which in particular includes values outside of \([2,8]\). For square ice, \(\kappa = 12\), which corresponds to \(c = -7\). The square ice Peano curve joins a tiny pantheon of models (including the uniform spanning tree and the Ising model) that have independently solvable random lattice analogs; these analogs are described in Ref. [21], along with connections to Liouville quantum gravity and string theory.
loop has weight \( r^4 + r^{-4} = n \). Thus
\[ n = C^2 - 2 \]  
and hence \( n = -2\Delta \).

The \( O(n) \) model loops are widely believed to be described by the conformal loop ensemble \( \text{CLE}_\kappa \) (the loop version of SLE), where
\[ n = -2\cos(4\pi / \kappa) \]  
[20]. [Here \( \kappa \) is a mnemonic for \( O(n) \).] The SLE-parameter for the Peano curve coming from the associated six-vertex model we call \( \kappa' \). Interestingly, \( \kappa' \neq \kappa \).

## IV. SIX-VERTEX HEIGHT FUNCTION VARIANCE

The variance in the height function of the six-vertex model was computed by Nienhuis [24]: When the height function \( h \) is measured in radians, for small \( a \), \( \exp(ia[h(x) - h(0)]) = \exp(-a^2/g \log |x|) \), where \( g \) is the Coulomb gas coupling constant. So the height variance, given by the quadratic term (in \( a^2 \)), is \((1/g) \log |x|\). From Ref. [24, (3.29)] we have
\[ \sin \frac{\pi g}{8} = \frac{C}{2} \]  
(5)

The theory of imaginary geometry, as developed by Miller and Sheffield, associates to a Gaussian free field (GFF) a space-filling SLE [8,25–27]. Roughly speaking, the GFF height function \( h \) is divided by a parameter \( \chi \) to obtain a field of orientations (measured in radians), and the orientation of the SLE curve is \( e^{ih/\chi} \). Thus the Coulomb gas coupling constant \( g \) and the parameter \( \chi \) (heuristically) related by \( g = \chi^2 \).

The space-filling SLE parameter \( \kappa' \) and \( \chi \) are related by
\[ \chi = \frac{\kappa'}{2} - \frac{2}{\sqrt{\kappa'}} \]  
[8], so
\[ \frac{1}{g} = \frac{1}{\chi^2} = \frac{4\kappa'}{(\kappa' - 4)^2}. \]  
(6)

If we parametrize \( n \) by \( n = -2\cos \theta \) with \( 0 \leq \theta \leq \pi \), then (2), (3), (5), (6), and (1) can be expressed as
\[ n = -2\cos \theta, \]
\[ \Delta = -\cos \theta, \]
\[ C^2 = 2 - 2 \cos \theta, \]
\[ \chi^2 = g = 4\theta / \pi, \]
\[ \kappa' = 4 + 8\theta / \pi + 8\sqrt{\theta / \pi + \theta^2 / \pi^2}, \]
\[ c' = 1 - 24\theta / \pi, \]  
(7)

where \( c' \) is the central charge associated with \( \text{CLE}_{\kappa'} \).

The table below gives some special cases. The limiting case \( C \to 0 \) is included, but with \( C = 0 \) the discrete models do not converge to SLE. Square ice is the \( C = 1 \) row. The special value \( C = \sqrt{2} \) is the “free fermion” point, where there is a mapping between the six-vertex model and square-lattice dimers; in this case \( \kappa' = 8 + 4\sqrt{3} \).
VI. MONTE CARLO SIMULATIONS

We used Monte Carlo simulations to check that the six-vertex model Peano curve is described by SLE$_\kappa'$. We produced six-vertex configurations on an $L \times L$ torus for various values drawn in blue in Fig. 2(b). The analogous “NW-tree,” which is the SE tree for the bipolar orientation obtained by reversing all the arrows, is drawn in red in Fig. 2(c). The SE tree and NW tree do not cross each other, so there is a curve winding between them, which is shown in green in Fig. 2(d). This map from bipolar orientations to Peano curves was first described for general planar graphs in Ref. [21]. This Peano curve is the same curve defined by the six-vertex height function.

Figure 3 shows a random sample of the Peano curve associated to a large square ice configuration on the square grid. For planar graphs, perfect samples for the six-vertex models with $C \geq 1$ can be obtained from single-site Glauber dynamics and coupling from the past [28].
We estimated the winding angle variance coefficients and the outer boundary dimension using samples for \(L = 256\) and \(L = 512\), as shown in Fig. 4.

The estimates for the winding angle variance coefficient is an excellent fit to the predicted value. Since the formula relating \(k'\) to \(C^2\) was derived from Nienhuis’s formula (5), the left panel of Fig. 4 is essentially an experimental verification of Nienhuis’s formula.

The outer boundary winding angle variance and dimension estimates (middle and right panels of Fig. 4) are both independent tests of the curve’s convergence to SLE. The estimated values are a close match to the predicted value, though when \(C^2 \approx 3.5\), the measured dimension deviates from the prediction by as much as 0.015. Further tests of the distribution of the loop length \(\ell\) and its dependence on \(L\) suggest that the convergence to the asymptotic behavior occurs for larger values of \(L\) when \(C^2 \approx 4\) than when, for example, \(C^2 \approx 2\). Overall, the experiments are consistent with convergence to SLE.

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