Aperiodic Ising models and low T Pinwheel tiling numerical expansion

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We calculate the low temperature expansion of free energy, heat capacity, and susceptibility in the Ising model embedded on the aperiodic Pinwheel tiling. The estimates are calculated for the 18 lowest terms in inverse bond strength and magnetic field strength. No directly consequential results are obtained from this work alone, but further steps are discussed.

I. INTRODUCTION

The mathematical simplicity of the Ising model [1] makes it approachable both numerically and analytically. Simultaneously, it is very potent in capturing the critical behavior, especially in the magnetic systems it is applied to. One class of systems that has garnered interest is aperiodic tilings, partially because they are geometrically similar to quasicrystals [2].

One aspect of interest in aperiodic tilings is how bond irregularity affects critical behavior. This phenomenon is captured by the heuristic argumentation of the Harris criterion [3].

In section II, we provide an intuitive derivation of the Harris criterion, and briefly discuss its relevance. In section III, we review work done on aperiodic tilings and introduce the Pinwheel tiling. We establish a way to computationally estimate the expansion coefficients for a general tiling. Estimates of the lowest order coefficients in a low T expansion are calculated in Pinwheel tiling for free energy, heat capacity, and susceptibility. Discussion about further improvements is provided.

II. MOTIVATION - THE HARRIS CRITERION

The simplest case of a d-dimensional Ising model consists of binary random variables $\sigma_i \in \{-1, 1\}$ on the sites i of a hypercubical lattice such that:

$$-\beta\mathcal{H} = \sum_{<i,j>} K\sigma_i\sigma_j + \sum_i h\sigma_i \tag{1}$$

where the notation $< i, j >$ means that the sum is taken over nearest neighbors.

In 1974, Harris considered the case of a lattice in which irregularity is introduced by randomly "breaking" some bonds, i.e. removing the interaction between the two sites [3]. Consider a system in which whether a particular bond between sites i and j is connected is determined by an independent Bernoulli random variable. The probability to be connected is $1 - p$. This leads to a concentration x of unconnected bonds, with $\langle x \rangle = p$

Similar to the derivation of the scaling hypothesis [4], we notice that the system is subdivided into independent volume elements Ω, whose characteristic size is:

$$\Omega \sim \xi^d \tag{2}$$

Since the bond breakings are independent Bernoulli random variables, the number n of missing bonds in an independent volume element Ω has the following second cumulant:

$$\langle n^2 \rangle_c = d\Omega p(1-p) \sim \xi^d x(1-x) \tag{3}$$

Thus the concentration fluctuations scale as:

$$\Delta x \sim \frac{\sqrt{\langle n^2 \rangle_c}}{\Omega} \sim \xi^{-\frac{d}{2}} \sqrt{x(1-x)} \tag{4}$$

If we assume that the function $T_c(x)$ is differentiable and non-zero, then for small Δx:

$$\frac{\Delta T_c}{T_c} \sim \Delta x \tag{5}$$

Now we get to the crucial part of Harris' argument. For the existence of ξ to be self-consistent, for large values the correlation length must scale at most as [3]:

$$\xi \leq \xi_0 \Big(\frac{|T - T_c(x)|}{T_c(x)} \Big)^{-\nu(x)} \tag{6}$$

Where we note that the critical temperature $T_c(x)$ and the critical exponent $\nu(x)$ are functions of x. Combining (6), (4), and (5), we get that the scaling must obey:

$$\xi^{1-\frac{d\nu}{2}} \leq A(x(1-x))^{-\frac{\nu}{2}} \tag{7}$$

for some A.

This now gives rise to the Harris criterion: for the fixed point to be stable, the LHS of (7) must be bounded for large ξ, implying: $d\nu < 2$. Using Josephson's identity $\alpha = 2 - d\nu$ [4], we retrieve the Harris criterion:

$$\alpha < 0 \tag{8}$$

Later in the 1970s, it was shown through RG calculations that if the Harris criterion is violated in an irregular system (i.e. $\alpha > 0$), the system's critical point can be changed [5], [6], [7] with critical exponents that differ from the universality class of the d-dimensional hypercube Ising model.

One obvious object of interest is now $d = 2$. The square Ising model in 2D is exactly solved, originally by Onsager in 1944 [8]. The results following the formulation of the Harris criterion hints that there might be other universality classes in $d = 2$ for lattices that are irregular. One hypothesized way such irregularity could be achieved is in the case of aperiodic tilings [9], which we investigate in the following section.

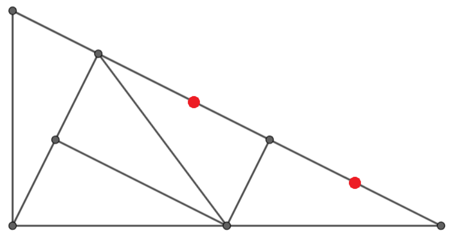

FIG. 1. The Pinwheel tiling generation. Dots indicate lattice points and lines their connectivity. Note that further iterations will add nodes to some bases of triangles, marked with red dots.

III. PINWHEEL TILING

The most notorious aperiodic tiling, Penrose Tiling, has already been quite thoroughly explored through Monte Carlo simulations [10], RG calculations [11], analytical calculation of series expansion coefficients [12], and numerical estimation of series expansion [9]. The work shows that the universality class of Penrose tiling is the same as for the standard 2d square lattice [9].

In this section, we investigate on the Pinwheel tiling [13] which, according to our best knowledge, has not been studied before in the context of Ising models. The study of the lattice is not directly motivated by a physical system. As can be seen in Fig. 1, the bond lengths vary greatly. Therefore it is not reasonable to think of the system as a directly magnetic one. Nonetheless, it is feasible to have more general networks resembling this shape, which have behavior captured by the Ising model.

A. Tiling definition and generation

We generate a Pinwheel tiling iteratively through the iteration procedure described in [13], in which an area in the shape of a right triangle, side lengths $1, 2, \sqrt{5}$, is repeatedly patched onto itself as in Fig. 1. The number of iterations m was varied between $m = 4, ..., 7$.

There is evidently some minor error in the code for generating the graph corresponding to the tiling, because the generations after 4 are no longer planar, and also include a non-extensive number of nodes whose coordination number is 14 and 15. This cannot represent the real tiling, since the geometry limits the coordination number to $\lfloor 2\pi/\tan^{-1}(1/2)\rfloor = 13$. However, the visual representation of the graph corresponds to the Pinwheel tiling for generations 1, 2, and 3, for which the overview is still relatively simple to do (fig 1 corresponds to generation 1). In the interest of time, we hope that this mistake does not have noticeable consequences to the statistical analysis.

B. Low-T expansion

Low-T expansion of the partition function is calculated by considering spin-flip excitations to the ground state as described in [14]:

$$Z = e^{\sum_r \frac{r}{2} g_{r,1} K} e^{Nh} \sum_{r,n} g_{r,n} e^{-2rJ} e^{-2nh} \tag{9}$$

where r is the number of "unsatisfied" bonds with opposite spins, which can be calculated using the coordination numbers of the nodes with spin-flips. n is the number of flipped spins, contributing to the magnetic field term in (1). The degeneracy term $g_{r,n}$ denotes the number of ways the tuple (r, n) can be included in the graph. Here the nearest-neighbor condition $< i, j >$ is understood as adjacency in the graph as illustrated by the edges in Fig. 1.

Taking the logarithm of (9), we get the negative of intensive free energy:

$$\frac{\ln Z}{N} = \overline{r}K + h + \ln\left\{1 + \sum_{r,n\neq 0,0} g_{r,n} x^r y^n\right\} \tag{10}$$

where we defined $x = e^{-2K}$, $y = e^{-2h}$, $\overline{r} = \sum_r r g_{r,1}/(2N)$. We can use the usual Taylor expansion for the logarithm in (10) to get the series:

$$\frac{\ln Z}{N} = \overline{r}K + h - \frac{1}{N}\sum_{k=1}^{\infty}\frac{(-1)^k}{k}\Big(\sum_{r,n\neq 0,0} g_{r,n} x^r y^n\Big)^k \tag{11}$$

Here we must note that the exact methods that were available for regular lattices no longer apply. The contributions $g_{r,n}$ are not a priori regular. Thus, we have the most general form of the expression as:

$$\frac{\ln Z}{N} = \overline{r}K + h + \sum_{r,n\neq 0,0} a_{r,n} x^r y^n \tag{12}$$

where $a_{r,n}(\{g_{r'\leq r,n'\leq n}\}, N)$ is a function of the lesser degree terms as defined by opening the parentheses in (11). In the thermodynamic limit $N \to \infty$, only the extensive terms in $l_{r,n}$ should contribute [14], and the $a_{r,n}$ thus become independent of N.

We calculate $g_{r,n}$ from the generated finite graphs directly using the Python Networkx library. This is done by exactly calculating the number of possible spin-flip contributions in the finite graph. The nodes at the perimeter, i.e. the largest triangles are excluded from the calculations of both the total node number N and the flips in degeneracies $g_{r,n}$, since they do not represent the bulk of the sample.

The low-T expansion could only be calculated to order $x^{10}y^3$ due to the fact that values beyond three flips become very time-consuming to calculate, even for only

$m = 4$. The smallest contribution from three separated spin-flip islands is $3 \cdot 3$, following from the smallest possible coordination number being 3, as can be seen in Fig 11. The calculated values for $a_{r,n}$ are presented in the following table. We make no quantitative claim about the precision of the numeric estimates:

m	4	5	6	7
N	425	2305	11640	58692
$a_{3,1}$	0.482	0.456	0.455	0.453
$a_{4,1}$	0.202	0.198	0.199	0.199
$a_{5,1}$	0.018	0.024	0.027	0.029
$a_{5,2}$	0.084	0.085	0.087	0.088
$a_{6,1}$	0.042	0.047	0.048	0.050
$a_{6,2}$	-0.020	-0.020	-0.021	-
$a_{7,1}$	0.014	0.017	0.019	0.019
$a_{7,2}$	-0.275	-0.252	-0.247	-
$a_{7,3}$	0.002	0.003	0.004	0.005
$a_{8,1}$	0.205	0.199	0.204	0.204
$a_{8,2}$	-0.035	-0.030	-0.032	-
$a_{8,3}$	0.030	0.015	-	-
$a_{9,1}$	0.028	0.028	0.029	0.029
$a_{9,2}$	-0.002	-0.004	-0.000	-
$a_{9,3}$	48.6	-	-	-
$a_{10,1}$	0.007	0.007	0.008	0.008
$a_{10,2}$	0.496	0.462	0.475	-
$a_{10,3}$	20.9	-	-	-

The dashes denote values that were omitted for the purposes of this paper, because the calculations were too time-consuming. In general the values behave non-extensively, apart from the calculated 3-flip terms $a_{9,3}$ and $a_{10,3}$, which have values $\gg 1$. We assume that this results from the sample being too small.

C. Low-T behavior of physical quantities

We may now infer the Low-T behavior of various physical quantities. Using the expressions for zero-field energy per site [14]:

$$\frac{E}{N} = -\frac{\partial}{\partial \beta}\Big(\frac{\ln Z}{N}\Big) \tag{13}$$

using the convention before for x and y, and $K = J\beta$ $h = H\beta$ we note:

$$\frac{\partial}{\partial \beta}x^r = J\frac{\partial}{\partial K}x^r = Jrx^{r-1}\frac{\partial}{\partial K}e^{-2K} = -2Jrx^r \tag{14}$$

$$\frac{\partial}{\partial \beta}y^n = H\frac{\partial}{\partial h}y^n = Hry^{n-1}\frac{\partial}{\partial h}e^{-2h} = -2Hny^n \tag{15}$$

where we used. Thus, the most general form in terms of expansion (12) is:

$$\frac{E}{N} = -J\Big(\overline{r} - 2\sum_{r,n\neq 0,0} a_{r,n} r x^r y^n\Big) - H\Big(1 - 2\sum_{r,n\neq 0,0} a_{r,n} n x^r y^n\Big) \tag{16}$$

The heat capacity could easily be derived for the more general case of finite H as the T-derivative of (16). For simplicity, the zero-field low-T heat-capacity is [14]:

$$\frac{C}{Nk_B} = 4K^2 \sum_{r,n\neq 0,0} r^2 a_{r,n} x^r \tag{17}$$

$$\frac{C}{4K^2 Nk_B} \approx 4.08x^3 + 3.18x^4 + 2.93x^5 + 1.08x^6 - 10.93x^7 + 11.97x^8 \tag{18}$$

where we truncate the series at x^8 since we do not claim to understand the contributions of $a_{9,3}$ and beyond. The value of $a_{r,n}$ is taken for the largest computed graph.

Likewise, we can calculate zero-field susceptibility:

$$\chi(x) = \frac{1}{N}\frac{\partial}{\partial H}\frac{\partial \ln Z}{\partial h}\Big|_{h=0} = 4\beta \sum_{r,n\neq 0,0} n^2 a_{r,n} x^r \tag{19}$$

$$\frac{\chi(x) k_B T}{4} \approx 0.45x^3 + 0.20x^4 + 0.38x^5 - 0.03x^6 - 0.97x^7 + 0.21x^8 \tag{20}$$

D. Possibility of estimation of critical exponents

Although the produced low-T expansion is short, we can try to estimate critical exponents using it. This can be done through Padé approximants. We conjecture that the system has a finite temperature critical point x_c and a general thermodynamic quantity $\Phi(x)$ behaves in its vicinity as [15]:

$$\Phi(x) \simeq A(x)\Big(1 - \frac{x}{x_c}\Big)^{\alpha} \tag{21}$$

This results in asymptotic behavior [9] [15]:

$$\lim_{x\to x_0}(x - x_0)\frac{\partial}{\partial x}\ln(\Phi(x)) = \alpha \tag{22}$$

We would in principle be able to provide a naive estimation of the critical exponents α and γ, governing the heat capacity and susceptibility respectively, from the expansions (18) and (19). However, the points at which either of these approximations gain finite value are $x_c = 0$ corresponding to the zero temperature limit, and $x_c \approx 1.27$, which corresponds to an antiferromagnetic interaction. Therefore, if a critical point exists for ferromagnetic interaction, which is the most likely scenario, our series is too short to capture the critical behavior.

E. Discussion

The work could be extended to higher order approximations with sufficient computational resources. The inclusion of k independent spin-flips increases the complexity to the order $O(N^k)$. The next large threshold happens for $k = 4$, which arises for terms with number of unsatisfied bonds $r \geq 12$. As seen in the behavior of terms $a_{9,3}$ and $a_{10,3}$, the size N cannot be made arbitrarily small without anomalies in the data. This naturally raises serious concerns about the time complexity for higher order coefficients.

Alternative approaches use more sophisticated methods, such as the recursive transfer-matrix method in [9] on a Penrose Tiling. However, these approaches require that the graph allows for moving a connected line across the majority of subgraphs in simple steps. In general, such approaches cannot be applied to an arbitrary graph. The simple computational approach demonstrated in this paper is not contingent on the type of graph, other than through the assumption that the finite size graph used is statistically representative of the whole system.

IV. CONCLUSION

According to the Harris criterion and subsequent work, 2d aperiodic lattices can in principle give rise to Ising models whose universality class is different than that of square Ising model. We examined an Ising model embedded on the aperiodic Pinwheel tiling. The lowest order expansion coefficients for free energy, specific heat, and susceptibility were calculated. Further work is required to make definitive statements about the critical behavior, but the methodology is verified to yield sensible results for the low order terms.

[1] E. Ising, Beitrag zer theorie des ferromagnetismus, Zeitschrift für Physik **31**, 253 (1925).

[2] M. B. U. Grimm, Aperiodic ising models, NATO ASI Series C **489**, 199 (1997).

[3] A. B. Harris, Effect of random defects on the critical behaviour of ising models, J. Phys. C: Solid State Phys. **7**, 1671 (1974).

[4] M. Kardar, The scaling hypothesis, in *Statistical Physics of Fields* (Cambridge University Press, 2007) p. 54–72.

[5] A. B. Harris and T. C. Lubensky, Renormalization-group approach to the critical behavior of random-spin models, Phys. Rev. Lett. **33**, 1540 (1974).

[6] T. C. Lubensky, Critical properties of random-spin models from the ϵ expansion, Phys. Rev. B **11**, 3573 (1975).

[7] G. Grinstein and A. Luther, Application of the renormalization group to phase transitions in disordered systems, Phys. Rev. B **13**, 1329 (1976).

[8] L. Onsager, Crystal statistics. i. a two-dimensional model with an order-disorder transition, Phys. Rev. **65**, 117 (1944).

[9] P. Repetowicz, Finite-lattice expansion for the ising model on the penrose tiling, J. Phys. A: Math. Gen. **35**, 7753 (2002).

[10] Y. Komura and Y. Okabe, High-precision monte carlo simulation of the ising models on the penrose lattice and the dual penrose lattice, Journal of the Physical Society of Japan **85**, 044004 (2016), https://doi.org/10.7566/JPSJ.85.044004.

[11] G. Xiong, Z.-H. Zhang, and D.-C. Tian, Real-space renormalization group approach to the potts model on the two-dimensional penrose tiling, Physica A: Statistical Mechanics and its Applications **265**, 547 (1999).

[12] P. Repetowicz, U. Grimm, and M. Schreiber, Planar quasiperiodic ising models, Materials Science and Engineering: A **294-296**, 638 (2000).

[13] C. Radin, The pinwheel tilings of the plane, Annals of Mathematics **139**, 661 (1994).

[14] M. Kardar, Series expansions, in *Statistical Physics of Fields* (Cambridge University Press, 2007) p. 123–155.

[15] S. Gluzman, Padé and post-padé approximations for critical phenomena, Symmetry **12**, 10.3390/sym12101600 (2020).

[16] M. R. E. S. Sørensen, M. V. Jaric, Ising model on the penrose lattice: boundary conditions, Phys. Rev. B **44**, 9271 (1991).

[17] N. G. de Bruijn, Algebraic theory of penrose's non-periodic tilings of the plane. i, Proc. K. Ned. Akad. Wet. Ser. A **84**, 39 (1981).