Statistical Mechanics, Three-Dimensionality and NP-completeness *

I. Universality of Intractability for the Partition Function of the Ising Model Across Non-Planar Lattices

[Extended Abstract]

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Dedicated to the memory of Professor Gian-Carlo Rota and Dr. Fred Howes.

ABSTRACT

This work provides an exact characterization, across crystal lattices, of the computational tractability frontier for the partition functions of several Ising models. Our results show that beyond planarity computing partition functions is NP-complete. We provide rigorous solutions to several working conjectures in the statistical mechanics literature, such as the Crossed-Bonds conjecture, and the impossibility to compute effectively the partition functions for any three-dimensional lattice Ising model; these conjectures apply to the Onsager algebraic method, the Fermion operators method, and the combinatorial method based on Pfaffians. The fundamental results of the area, including those of Onsager, Kac, Feynman, Fisher, Kasteleyn, Temperley, Green, Hurst and more recently Barahona:
• for every Planar crystal lattice the partition functions for the finite sublattices can be computed in polynomial-time, paired with the results of this paper:
• for every Non-Planar crystal lattice computing the parition functions for the finite sublattices is NP-complete, provide an exact characterization for several of the most studied Ising models. Our results settle at once, for several models, (1) the 2D non-planar vs. 2D planar, (2) the next-nearest neighbour interactions vs. 2D, and (3) the general 3D Ising, intensively studied open problems of the area.

Our results are obtained by establishing a Kuratowski-like charcterization theorem for the class of (infinite) crystal lattices called Bravais lattices, that can also be extended to general crystal structures. The "forbidden subgraph," called *Kuratowskian*, plays the central role, being contained in every non-planar crystal lattice. This *universality* phenomenon (existence independent of lattice structure), captured in the "equation": Translational Invariance + Non-Planarity = Universality of Subgraphs, provides a unified understanding of non-planarity as a root of computational intractability. The important structural property of the Kuratowskians is that they are "embedding-universal" for 3-regular graphs, in the sense that every such graph has a subdivision included in the Kuratowskian. Several NP-hardness results are obtained in this paper, by using different types of Kuratowskians, which in turn witness NP-hardness of various counting coefficients of the partition functions.

The exceedingly complex mathematical methods that solved the planar cases of the Ising model, could be interpreted as an explanation of why no 3D solvable cases have been found. Richard Feynman in 1972 commented *" The exact solution for three dimensions has not yet been found"*. Our results, for the Ising models that we consider in this paper, provide evidence of a paradigm-shift: the *"has not yet been found"* needs now be replaced with *"it may be computationally intractable across lattices."*

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1. INTRODUCTION

1.1 The Search for Exactly Solved Models in Statistical Mechanics

One of the most exciting periods in statistical mechanics was in 1944, with the discovery by Lars Onsager of the first exactly solved model that exhibits a provable phase transition. The model was the Ising model of ferromagnetism on the two-dimensional square lattice. This result energized some of the most brilliant researchers, both physicists and mathematicians in the quest for generalizing the method and carrying on the search for other exactly solved models, towards the three-dimensional models. Decades of research of highest distinction uncovered new methods, and focused on a variety of lattices in the search for other tractable models. The research eventually was extended to rigorously solve all planar lattices, but no three-dimensional lattice was found to be exactly solvable. All methods proposed, from Onsager's, to Fermions, and to Pffafians, were all rediscovering the same tractable planar cases, and none could deal with the 3D case. Tractability was hitting a "wall" no matter what methods were used. Even research focusing on 2D nonplanar lattices, of significant interest in statistical physics, turned out without success. Non-planarity of the lattice, expressed in physical terminology as lattices with "crossed-bonds", was observed to be the root of difficulty for various methods. The search for understanding the limitations of the methods based on Onsager, Fermions and Pfaffians continued to be active for several decades.

In this work we identify the exact computational tractability frontier of these methods in the context of some of the most studied variants of the Ising model. Here [1] are citations due to some of the major research contributors of the area, recording both excitement and hopelessness about the state of the research in early 70's; with the today knowledge on computational complexity, we can see that these comments describe the simptoms of an NP-completeness phenomena.

1.2 The Two Dimensional Ising Model

Exactly solved models in statistical mechanics are few [2], and all are one- or two-dimensional lattice models; the most fundamental of them is the two-dimensional Ising Model of Ferromagnetism, exactly solved by Onsager. The importance of such exact solutions is due to the physical insight they provide into phase transitions. The solution provides an analytical closed-form/or rigorously solved form for the partition function, which in turn provides the basis for exact predictions for such systems: all thermodynamical quantities can be computed exactly.

The Ising model was introduced by Ernst Ising in 1925 [18]. In 1936, Peierls [33] showed by a probabilistic argument that the two-dimensional Ising model has a phase transition. In

[1] H. N. V. Temperley wrote in 1974 [35] *No physically interesting non-planar lattice has been solved completely as yet... The simplest such lattice is the plane square lattice with interactions along the diagonals as well as the sides of the squares (sometimes called the "union jack" lattice)... It is somewhat melancholy thought that nearly twenty further years of work has added relatively little to our knowledge of* anlytical *properties of the Onsager-ising model itself, though we now have a great deal more information deduced from series expansions. ... With monotonous regularity each method has reproduced virtually the same results as those listed above and has added virtually no new ones on the analytic side. This information may be summarized as knowledge for planar lattices, but not for any interesting non-planar lattice, of the partition function and correlations as a function of temperature in zero magnetic field, together with the spontaneous magnetization and various boundary and impurity effects. ... It relates either the trace of "vacuum to vacuum expectation" of a product of linear sums of operators, known as Clifford or Fermi operators, to what is known mathematically as a Pfaffian. This experience is almost unique in mathematical physics. (Nearly always a valid new treatment of a problem produces new results as well as repoducing old ones.)*
McCoy and Wu wrote in 1973 [28] in the comprehensive monograph *The Two-Dimensional Ising Model* at the end of the book:
Conspicuously missing from the table of open problems are: (1) the calculation of the free energy of the two dimensional Ising model when $H \neq 0$, and (2) the calculation of the free energy of the three dimensional Ising model. This omission is intentional. *These two problems are both extremely difficult. Indeed, they have existed for a quarter of a century and absolutely no progress has been made. (By no progress, we mean no progress toward an explicit solution).*
Mark Kac in 1985 [22]
The three-dimensional case does exhibit a phase transition but exact calculation of its properties has proved hopelessly difficult. The two-dimensional case for so-called nearest-neighbour interactions was solved by Lars Onsager in 1944. Onsager's solution, a veritable tour de force *of mathematical ingenuity and inventiveness, uncovered a number of suprising features and started a series of investigations which continue to this day.*
The solution was difficult to understand and George Uhlenbeck urged me to try to simplify it. "Make it human" was the way he put it. ... At the Institute [for Advanced Studies at Princeton] I met John C. Ward ... we succeding in rederiving Onsager's result. Our success was in large measure due to knowing the answer; we were, in fact, guided by this knowledge. But our solution turned out to be incomplete ... it took several years and the effort of several people before the gap in the derivation was filled. Even Feynman got into the act. He attended two lectures I gave in 1952 at cal Tech and came up with the clearest and sharpest formulation of what was needed to fill the gap. The only time I have ever seen Feynman take notes was during the two lectures. Usually, he is miles ahead of the speaker but following combinatorial arguments is difficult for all mortals.
Richard Feynman in 1972 [7]:
The exact solution for three dimensions has not yet been found.
C. A. Hurst in 1965 [17]:
" It has been rather puzzling that the two methods at present known for finding exact solutions for the Ising problem, namely the algebraic method of Onsager and the combinatorial method emplying Pfaffians, have exactly the same range of application, although, they appear so different in approach. Problems which yield to one method yield to the other, whilst problems which are not tractable by one approach also fail to be exactly solved by the other, although the reasons for this failure appears to have completely different mathematical origins. On the one hand, Ising problems which cannot be solved by the Pfaffian method are characterized by the appearance or **crossed bonds** *which produce unwated negative signs in the combinatorial generating functions, and such crossed bonds are usually manifestations of the topological structure of the lattice being investigated, i.e., the three-dimensional cubic lattice. On the other hand, the Onsager approach breaks down because the Lie algebra encountered in the process of solution cannot be decomposed into sufficiently simple algebra. It is usually stated that such more complicated algebras occur only when the corresponding lattice has crossed bonds, although an explicit proof of this fact does not appear to be published. ... It is difficult to see why the two methods have exactly the same limitations ...*
P. W. Kasteleyn in 1967 [25]:
" The dimer problem and the Ising problem were finally solved for planar lattice graphs only, and it was found that a generalization to non-planar lattice graphs (including all three-dimensional lattice graphs) is impossible unless the number of Pfaffians involved is allowed to increase to intractably large numbers.

1941, Kramers and Wannier [26] established the exact location of the phase transition, the Curie point, based on the assumption that such a point is unique. Onsager, in 1944, [31] provided the complete, definitive exact solubility of the two-dimensional square lattice Ising model.

All such results were obtained using extremely complex mathematical arguments. A tremendous research effort in mathematical physics emerged for the identification of those crystal lattice structures that provide soluble models. New powerful mathematical methods were discovered, but none of them were able to identify any soluble three-dimensional model. However, the belief was that advances in mathematical physics will eventually solve such models.

As Onsager's solution was an extraordinarily deep and involved argument, George Uhlenbeck challenged Mark Kac to "Make it human" [22]. Kac and Ward in 1952 [23] attempted to provide an exact evaluation of Onsager's partition function formula based on a combinatorial interpretation. This is based on viewing the partition function as the generating function for the graph-counting problem of Eulerian subgraphs of the lattice. They reduced the problem to that of computing a determinant. The argument, however, was incomplete. Feynman [22] provided the key technical formulation of the needed missing lemma, the so-called Feynman's conjecture [13; 15], which eventually was proven by Sherman in 1960 [34], making the Kac-Ward method completely rigorous. A variant of the Kac-Ward method occured in the early 1960s, based on the Pfaffians. In this method, the same combinatorial interpretation is used, but the problem is reduced to a related problem of counting dimers in an associated lattice (or perfect matchings) which was solved using determinats via Pfaffians by Kasteleyn 1964 [**?**], and Fisher [8].

A more comprehensive account of the developments concerning statistical mechanics research of the Ising model can be obtained from: [6], [5], [8], [35], [20], [37], [30], [17], [29], [16], [4], [9], [27], [10], [3], [14], [28],

1.2.1 Ising Models and Computational Complexity

NP-completeness was used as a rigurous method to classify the computational complexity of problems in statistical physics, see e.g., [36; 37]. Powerful intractability results, previously obtained, in the area of Ising models, closely related to this research used different classes of graphs.

• *Graphs: Finite sublattices of a specific lattice.* Barahona [1] showed that for the Ising model on 3D cubic lattice, with interaction energy $\{-J, 0, +J\}$, the problem of computing the ground states on finite sublatices is NP-complete. Our work builds and extends the elegant work of Barahona, showing that computational intractability is present in every non-planar lattice, including the 2D non-planar lattices.

• *Graphs: The entire class of finite graphs.* Results by Jerrum and Sinclair [21], and Jaeger, Vertigan and Welsh [19] show that computing the partition function for the Ising model in this case is NP-complete.

1.3 An outline of the paper

The technical outline of the paper is as follows. First a Kuratowski-like charcterization theorem is proved for a class of (infinite) crystal lattices called Bravais lattice. Basically, the theorem is general and follows from the two "axioms" (1) translational invariance (of crystal lattices) and (2) non-planarity. The "forbidden subgraph" called *Kuratowskian* plays the central role in what follows. By the theorem it is contained in every non-planar crystal lattice. This *universality* phenomenon (existence independent of lattice structure) holds the key to the universality of NP-completeness of the partition functions of the Ising model for finite sublattices. The important structural property of the Kuratowskians is that they are embedding-universal for 3-regular graphs, in the sense that every such graph has a subdivision included in the Kuratowskian. This gives the fertile ground for a proof of NP-completeness. Several results are obtained in the paper, by using different types of Kuratowskians, which in turn show NP-hardness of various counting coefficients of the partition functions.

2. ISING MODELS

Ising models are of fundamental importance in statistical physics. The Ising model can be formulated on any graph as follows. Consider a graph $G_N = (V, E)$, having N *vertices* (representing lattice sites) $V = \{v_1, ..., v_N\}$, and a set E of *edges* (representing the near-neighbour interactions). Each edge $(i, j) \in E$ has an associated constant *interaction energy* or *coupling constant* J_{ij} is a positive, zero or negative number. We interpret J_{ij} as labels of the corresponding edges. The model is usually defined as the the graph of a crystal lattice where the vertices represent *lattice sites*, and the edges represent *near-neighbour interactions*.

Every vertex v_i has a magnetic *spin* variable σ_i associated with it; it takes values $\sigma_i = \pm 1$, where $+1$ represents the "up spin", and -1 represents the "down spin". A *state* or a *spin configuration* ω is an assignment of N ± 1 values to the variables $\sigma_i, 1 \leq i \leq N$. Let $\Omega = \{-1, +1\}^N$ be the set of all spin configurations.

The *energy* of a state ω in zero magnetic field is given by the Hamiltonian: $H(\omega) = -\sum J_{ij}\sigma_i\sigma_j$. Three fundamental objects of study for statistical physics are:

Ground State A spin configuration of minimum energy is called a ground state.

Partition Function The partition function of the Ising model is given by:

$$Z(\omega) = \sum_{\omega \in \Omega} e^{-\frac{H(\omega)}{\kappa T}}$$

where κ is the Boltzmann constant, and T is the temperature.

Free Energy The free energy from the magnetic degree of freedom is $\kappa T \log Z(T)$, and the equilibrium magnetic properties, magnetization, entropy, magnetic energy, specific heat and susceptibility, can all be obtained by differentiating the partition function with respect to the temperature.

In this first paper we will be concerned with the problems of computing ground states and partition functions. We will not address directly the problem of computing the free energy.

2.1 Ground States and the Minimum Weight Cut

Let us consider a graph $G_N = (V, E)$ with its edges weighted by the J_{ij} interaction energies. The energy of a state $\omega = (\sigma_1, ..., \sigma_N)$ is given by $H(\omega)$. It is easy to see that H can be defined in terms of *cuts* in G_N. Indeed, for a state $\omega = (\sigma_1, ..., \sigma_N)$, let us denote by $C^+ = \{v_i \mid \sigma_i = +1\}$, and by $C^- = \{v_i \mid \sigma_i = -1\}$. This defines the *cut* $C = (C^+, C^-)$ of G_N. Let us also define E^+, and E^- as the set of edges with both endpoints in C^+, and respectively in C^-. We divide the vertices in two parts. The cut refers to the set of edges that cross between the "up spins" vertices to the "down spins" vertices. Let E^{+-} be the set of edges in the cut, that is, all edges with one endpoint in the C^+ and the other in C^-. Another alternative notation for E^{+-} that highlights the cut C is $\delta(C)$. The *weight* of the cut is $weight(C) = \sum_{ij \in \delta(C)} J_{ij}$. The summations used in defining the model are over edges in the graph: the short hand ij stands for $\{v_i, v_j\}$.

Clearly as ω varies over all spin configurations, the corresponding cut C ranges over all cuts of G_N. Observing that we actually have a one-to-one correspondence between spin configurations and cuts we can write the Hamiltonian as follows: $H(C) = -\sum_{ij \in E^+} J_{ij} - \sum_{ij \in E^-} J_{ij} - \sum_{ij \in E^{+-}} J_{ij}$ and so $H(C) = -\sum_{ij \in E} J_{ij} + 2\sum_{ij \in \delta(C)} J_{ij}$. If C is the cut defined by ω, $H(\omega)$ is the same as $H(C)$. For a given cut, the Hamiltonian is now a sum of a constant term (for the graph) and twice the weight of the cut. Minimizing the Hamiltonian, that is, finding the ground state, is therefore, equivalent to computing the cut of minimum weight in our graph.

The *Minimum Weight Cut* Problem can be solved in polynomial time for the class of weighted planar graphs. That is, for every choice of positive, zero or negative weights for the edges of a planar graphs, we can compute in polynomial time the minimum weight cut of such graphs. The problem in NP-complete on arbitrary graphs.We will show in section **??** that the same problem is NP-complete for *every* non-planar crystal lattice graph, when restricted to the set of its finite sublattices.

3. PLANAR LATTICES: COMPUTATIONAL TRACTABILITY

Computing both the ground states and the partition function for planar graphs can be done in polynomial time, [1] and [27]. Planarity and its duality are fundamental for obtaining computationally tractable solutions. For the minimum weight cuts in planar graphs, algorithms are due to Hadlock 1975 [12] and Goodman and Hedetniemi [11], and [32]. The problem of computing the partition function for the zero field Ising model for finite planar lattices is equivalent to that of computing a determinant, and therefore, can be done in polynomial time. For planar graphs, *Pfaffian orientations* could be constructed (Kasteleyn's theorem [24], which in turn relate the underlying problems of counting cuts, to the problem of counting Eulerian subgraphs in the dual lattice, and therefore, to that of evaluating Pfaffians, which can be expressed in terms of determinants [1]. Our results from the section **??** show that unless $P = NP$ no such results can be extended to any non-planar crystal lattice.

4. NON-PLANAR LATTICES: COMPUTATIONAL INTRACTABILITY

Crystal lattices are defined in two stages: Bravais Lattices, and their generalizations, the crystal structures [**?**]. We will present in this extended abstract the details of the dvevelopments for non-planar Bravais lattices, and leave the description of their extensions to crystal lattices to the final version of the paper.

4.1 Bravais Lattices

Crystal lattices are defined in terms of Bravais sets of points. We are interested in such sets in the two-dimensional and three-dimensional space. A *d-dimensional Bravais lattice L* is the infinite set of points in the d-dimensional Euclidean space whose position vectors r are given by

$$r = x_1a_1 + x_2a_2 + ... + x_da_d$$

where $a_1, a_2, ..., a_d$ are linearly independent vectors, and $x_1, x_2, ..., x_d$ are integers. The *finite* $N_1 \times N_2 \times .... \times N_d$ sublattice of the infinite lattice L, denoted $L[N_1, ..., N_d]$, is obtained by imposing a boundary for every $x_i, 1 \leq i \leq N_i, 1 \leq i \leq d$. Interaction are specified as a set of pairs of points, typically near-neighbour. Line segments are drawn between two interacting lattice points. The lattice points are the vertices, and the interaction pairs define the edges of our lattice graphs.

4.2 Non-Planar Bravais Lattices

We will show that the computation of the ground states is NP-complete in every non-planar Bravais lattice.
We first give a charcterization theorem in the spirit of the Kuratowski theorem for planar Bravais lattices. The forbidden sublattice unvailed by the theorem, that we call the *Basic Kuratowskian*, has interesting properties. First of all, every non-planar Bravais lattice contains Kuratowskians, i.e., subdivisions of the Basic Kuratowaskian. Second, computing ground states on the Basic Kuratowskian is NP-complete; and the same property holds for any of its subdivision. These two facts establish our first main result.

We then focus on a more elaborate version of the Kuratowskians, called *uniform Kuratowskian.* We develop similar results using them. In turn, we use these structures to establish computational intractability of partition functions, where computing ground states is easy, but other components are NP-hard.

4.2.1 The Kuratowskians

The finite lattice graph in figure 1 plays a special role in this paper. It generically defines an infinite lattice graph. We call the inifinite graph the *Basic Kuratowskian*, and denote it by $\mathcal{K}_0$. It captures through its subdivisions, common structural characteristics present in each and every non-planar infinite Bravais lattice. We will use the term *Kuratowskian* for any subdivision of the Basic Kuratowskian.

DEFINITION 1. *We will call* Kuratowskian *every subdivision of $\mathcal{K}_0$.*

Let us remark that non-planarity for an infinite lattice means that one of its standard finite subgraphs is non-planar.

LEMMA 1. *The infinite Basic Kuratowskian $\mathcal{K}_0$ is a non-planar graph. Moreover, every Kuratowskian is non-planar.*

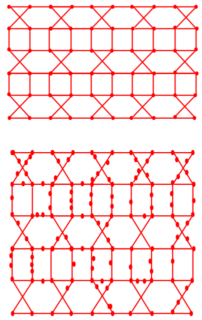

Figure 1: A finite sublattice of the Basic Kuratowskian $\mathcal{K}_0$ and a subdivision of it.

Proof. It suffices that a standard finite sublattice graph $\mathcal{K}_0$ is non-plnar. This means by the Kuratowski theorem that one such sublattice has as a subdivision one of the Kuratowski graphs, $K_{3,3}$ or K_5. Figure 4.2.3 shows a subdivision of $K_{3,3}$ contained in $\mathcal{K}_0$. Clearly, the same property is true for every subdivisions of $\mathcal{K}_0$. Each such subdivision will have a a finite sublattice graph that is non-planar.

We will show that every Bravais lattice contains Kuratowskians as sublattices. This will provide a unifying framework of a type of universality property with respect to the computational complexity of the partition functions for such lattices.

4.2.2 A Kuratowski-like Theorem for Bravais Lattices

In this section we give a necessary and sufficient condition for a Bravais lattice graph to be planar. The characterization, as in the Kuratowski Theorem, is in terms of forbidden subgraphs. Our Basic Kuratowskian plays the same role as the one played by the Kuratowski graphs $K_{3,3}$ and K_5.
Consider an infinite Bravais lattice L that is non-planar. Non-planarity implies that there is a standard finite sublattice graph A that is non-planar. By the Kuratowski theorem, A contains a subdivision of one of the Kuratowski graphs $K_{3,3}$ and K_5, say K. By translational invariance of the Bravais lattice, there are infinitely many disjoint copies (their sets of vertices are disjoint) of K in L. We will use such occurences of K to identify non-planar pieces, called *corssing gates*. Then we will interconnect these gates and will form a network that connects in a planar manner all these non-planar pieces. This construction will witness the containment of a Kuratowskian in L.

THEOREM 1. *A 2D or 3D infinite Bravais lattice is planar if and only if it does not contain the Basic Kuratowskian $\mathcal{K}_0$ or any of its subdivisions.*

Proof. Let us consider L an infinite Bravais lattice.
(1) Suppose first that L contains a Kuratowskian. Then, by the Lemma 1 it follows that L is a non-planar lattice graph.
(2) Suppose now that L is non-planar. To establish the other part of the theorem, we will show that for L there exists a specific subdivision of $\mathcal{K}_0$ that is contained in L. We treat the two cases 2D and 3D separately.

We will use pairs of (non-colinear, respectively, non-planar) vectors, defining the interaction pattern of the lattice, to construct corresponding "tesselation" planes in the lattice.

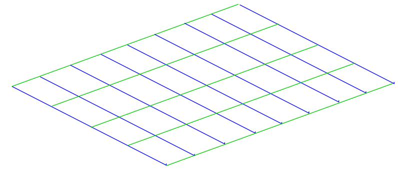

Figure 2: A "tesselation plane" of the Bravais lattice defined by two non-colinear vectors. It divides the plane into paralelograms.

Then, non-planarity of the L would imply existence of subdivisions of the Kuratowski subgraphs, that in turn will pinpoint to occurences of crossing pair of paths. The combination between tesselation planes and crossing pair of paths define a "Kuratowski network". This in turn contains a subidvision on $\mathcal{K}_0$.

• *L is a 2D Bravais lattice.*
Crossing paths. Let $\pi = \{\rho_1, \rho_2, ..., \rho_t\}$ be the interation pattern of L. Assume that L is embedded in the plane, with vertices drawn as points, and the edges as straight line segments connecting corresponding points. L being non-planar implies that some of the line segments cross; crossing could happen between two segments, or, one segment can cross a two segment path going through the middle vertex. We use the Kuratowski theorem to find crossing paths. The non-planarity of L implies that there is a standard finite sublattice $L_{N\times N}$ containing a subdivision of a graph $K \in \{K_5, K_{3,3}\}$. Let us fix that occurence of the subdivision of K in L. Because K is non-planar, there should exist four vertices of K, say v_1, v_2, v_3, v_4 and two paths P_1 and P_2 in K, such that: P_1 starts at v_1 and ends at v_2, and P_2 has end points v_3 and v_4, and P_1 crosses P_2 exactly once. Moreover, we chose the two paths such that they are minimal in size with respect to this property.
Tesselation planes. As the interaction pattern of a non-planar lattice graph needs to have at least 3 vectors, let us consider two vectors that are non-colinear, say, ρ, ρ' in π. Let T the corresponding tesselation of the 2D plane. *Crossing gates.* We will form such a "crossing gate" by using the two crossing paths P_1 and P_2 that we identified in K, and a paralelogram A in T that is large enough and contains P_1 and P_2 in the planar area that it defines. We pick A such that (1) we can extend P_1 and P_2 such that they become diagonal paths for A such that these extensions are contained inside A, using no edge segments from A's boundary. The resulting structure consisting of A together with the these crossing diagonal paths is called a *crossing gate*. Let us note that such a crossing path could be unique, but it must exist. Both $K_{3,3}$ and K_5 are non-planar, but could become planar if one one of their edge is removed. *Kuratowski Network.* Consider now an arrangement of these crossing gates as arranged in the figure 4.2.2. The crossing gates are connected using connecting paralelograms of T of appropriate size. We call the arrangement a *Kuratowski Network*. Note that the network connects in a planar way non-planar crossing gates. It is easy to see that this Kuratowski network contains a subdivision of $\mathcal{K}_0$. The crossing gates are arranged in a row and such rows alternate with rows with no gates. Therefore, L, contains a subdivision of $\mathcal{K}_0$.

• *L is a 3D Bravais lattice.*

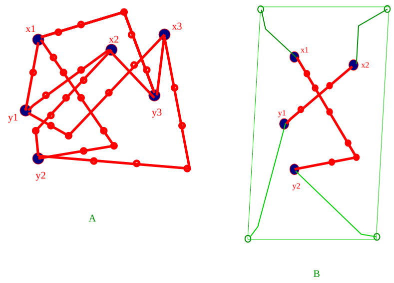

Figure 3: A: An occurence of a subdivision K of $K_{3,3}$ in a non-planar lattice; B: A pair of crossing paths given by K extended to a crossing gate within a paralelogram of a tesselation plane

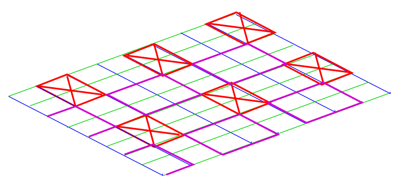

Figure 4: The Kuratowski Network in a 2D non-planar lattice

The proof is as before, with the exception that we are now in 3D, and a few things change. One is the fact that " paths crossing" is no longer well-defined. Therefore, we will consider two non-colinear vectors $\rho_1, \rho_2 \in \pi$, as before, and the teselation plane*s* T_i that they define. Consider K' a subdivision of a Kuratowski graph K, that is contained in L. K' is non-planar, and so is any "projection" on any tesselation plane T_i. Our crossing gates will be three-dimensional, while the interconnection between them will be two-dimensional planar.
Let us pick a tesselation plane T that is defined by non-colinear vectors ρ_1 and ρ_2 such that it has no vertices in common with K'. We will use a third vector $\rho_3 \in \pi$, that is not *co-planar* with the first two, to project the ends of a pair of crossing paths (as viewd crossing when projected to T) from K'.
We pick as before two crossing paths P_1 and P_2 in K' with end points v_1, v_2, and respectively v_3, v_4. Our choice of the crossing paths is such their four end points are projected into four points on T, using the ρ_3 lines for projection. We can always make this choice, if necessary shortening the paths and extending them with edges in the ρ_1 and ρ_2 directions. Let the projections of v_1, v_2, v_3, v_4 on T be v'_1, v'_2, v'_3, v'_4.
We will continue our construction as in the 2D case, by finding a paralelogram A of T that contains these four points and such that each of our crossing paths could be extended with segments interior to A to connect opposite corners of A. The paralelogram A and these diagonal paths form the new "crossing gates."
It is easy to see now, that we can use the plane T to connect the gates and to form a similar Kuratowski network for L. Figure 4.2.2 shows the generic construction. It is easy to see that a subdivision of $\mathcal{K}_0$ is contained in L having the "X" crosses partially, outside the plane T, where the "X"s are connected by a two-dimensional planar set of edges. Clearly, for a given non-planar lattice, the Kuratowski network is not unique.

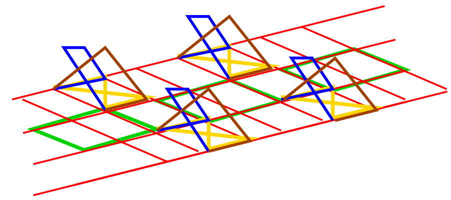

Figure 5: The Kuratowski Network in a 3D non-planar lattice

4.2.3 Universality of graph embedding into Kuratowskians

In this section we show that for every 3-regular graph, and for every Kuratowskian, there is one subdivision of the graph that is contained into the Kuratowskian.
Kuratowskians are universal for subdivisions of 3-regular graphs

The lattice $\mathcal{K}_0$ has the following "3-universality" property.

DEFINITION 2. *A lattice is called* 3-universal *if every 3-regular graph has a subdivision that is contained in the lattice.*

LEMMA 2. *$\mathcal{K}_0$ is 3-universal. Moreover, every Kuratowskian is also 3-universal.*

Proof. Figure 4.2.3 shows a subdivision of K_{33} contained in $\mathcal{K}_0$. We now present an algorithm that for every 3-regular graph $G = (V, E)$, will find a subdivision G' of G that will be contained in $\mathcal{K}_0$.
Suppose that $V = \{v_1, ..., v_n\}$ and $E = \{e_1, ..., e_m\}$. We will select a set of $3 * n$ columns in $\mathcal{K}_0$, three columns for each vertex of$G$. From left-to-right, the first three columns will be assigned to vertex v_1, the next three to vertex v_2 and so on. The vertices will be located in the middle column of the three columns associated to it. We will also select m X-rows, each corresponding to an edge of G. The first row of X-es will be assinged to e_1, the next to e_2 and so on. Each edge $e_k = (v_i, v_j)$ will be present as a subdivision, i.e., a path p_{e_k}, that will connect v_i with v_j. Suppose that $i \leq j$. The path p_{e_k} will use: (1) the column where v_i is located to start from v_i and to reach lower to the X-row assignated to the edge e_k; (2) it will continue on this row till it will reach the column where v_j is located; (3) finally, it will use this column to reach the vertex v_j. All these paths will be vertex disjoint regardless what the edge structure of G is. As expected, when such paths must cross, the X-gates will be used to accomodate this crossing whithout sharing vertices.

4.2.4 The Uniform Kuratowskians

A similar set of results can be obtained for a special type of Kuratowskian, called *uniform Kuratowskian.* They are going to play a similar role, by providing a Kuratowski-like characterization of non-planar lattices, and by provising again universality of embedding for 3-regular graphs. This time, however, the subdivisions of 3-regular graphs will be uniform, that is, all edges replaced by subdivisions of the

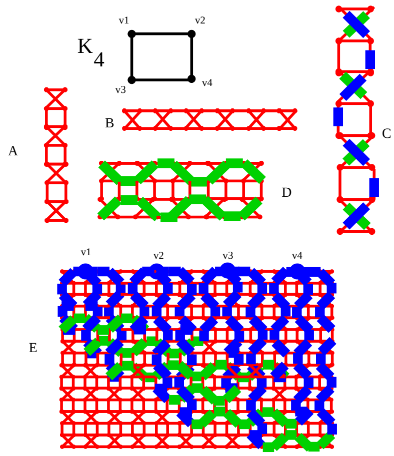

Figure 6: A subdivision of the graph K_4 contained in the basic Kuratowskian

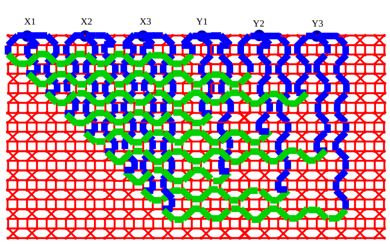

Figure 7: A subdivision of the graph K_{33} contained in the Basic Kuratowskian

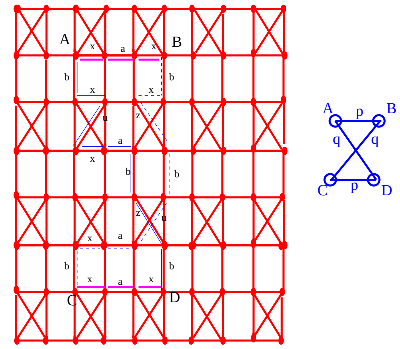

Figure 8: Construction of the uniform crossing gate

same length. The new construction is based on an *uniform crossing gate* that is presented in the Figure 8. Complete details will be presented in the final version of this paper.

5. COMPUTATIONAL COMPLEXITY OF THE 3D ISING MODELS

We will consider four cases: models with $\{-J, 0, +J\}$ interactions, with $\{-J, 0\}$ interactions, with $\{0, +J\}$ interactions, and with $\{-J, +J\}$ interactions. We will show that the computation of the partition function is NP-complete for all such cases when the crystal lattice is non-planar. However, as we restrict the type of interactions along these four models, the roots of computational intractability become deeper.

5.1 Ising Models with $\{-J, 0, +J\}$ Interactions

Recall that computing the lowest energy state, i.e., the ground state is equivalent with computing the cut of minimum weight, where the cut is defined by the edges that have their nodes associated opposite spins. We show that in this case, computing the ground state is NP-complete. We reduce the problem to that of computing the maximum cut in 3-regular graphs. The proof uses the containment, for every non-planar lattice of a Kuratowskian into the lattice.

THEOREM 2. *Consider the Ising model with interaction energies $\{-J, 0, +J\}$. For every non-planar crystal lattice, computing the Ground States of finite sublattices is NP-complete. Therefore, computing the Partition Functions for the finite sublattices is also NP-complete. NP-complete.*

Proof. Let us consider L a non-planar crystal lattice, and let $\mathcal{K}'$ be its Kuratowskian. Let us assign weight 0 to every edge of L that is not in $\mathcal{K}'$. As computing ground states on finite sublattices is now equivalent to computing the Minimim Weight Cut on $\mathcal{K}'$, it will suffice to show that this last task is NP-complete. This is established in lemma 3, which in turn establishes the theorem. The lemma and its proof are similar to what we can coin as the *Barahona Lemma*, [1].

LEMMA 3. *Computing Min Weight Cut on $\mathcal{K}_0$ with weights $\{-J, 0, +J\}$ is NP-complete. Moreover, the same is true for every subdivision of $\mathcal{K}_0$.*

Proof. By Lemma 2, for every 3-regular graph G there exists a subdivision G' of G that is contained in $\mathcal{K}_0$. Let us assign weight 0 to every edge of $\mathcal{K}_0$ that is not in G'. Consider one edge $e = (v_1, v_2)$ and the corresponding subdivision of e namely $p_e = (w_1, w_2, ..., w_{t+1})$ that is composed of the $t \geq 1$ edges. Label one edge picked arbitrarily by $-J$ and the rest of the edges by $+J$. We claim that there exists a cut in G of size $\geq h$ if and only if there exists a cut in (G', λ) of weight $\leq -hJ$. Indeed, Consider a cut $C = (S_1, S_2)$ in G of size r, and let E_C be the edges of the cut. Then it is easy to see how to construct a cut C' in (G', λ) of weight $-r$. Let $E_{C'}$ be the set of edges labeled $-J$ in all the paths p_e, where $e \in E_C$. Let C' be the cut defined by the edes $E_{C'}$ as follows. We define the cut (S'_1, S'_2) such that $S_i \subset S'_i$ in the obvious way. We have $w(C') = -tJ$. Conversely, let us observe that if there is a cut C' in G' of weight $-rJ$, and the cut edges are the only edges labeled $-J$ then there exists a cut in G of size r. However, if C' contains also edges labeled $+J$, it may not exist a cut is G of size exactly r, but it should exist one cut of larger size.

Therefore, as computing Max Cut for 3-regular graphs is NP-complete, it follows that computing the Minimum Weight Cut for $\mathcal{K}_0$ with labels $\{-J, 0, +J\}$ is NP-complete. It is easy to see that the same conclusion holds for every subdivision of $\mathcal{K}_0$, as 3-universality also holds for all subdivisions of $\mathcal{K}_0$.

5.2 Ising Models with $\{0, +J\}$ and $\{-J, 0\}$ Interactions

In this section we analyse the case of non-negative pairwise interactions for the $\{0, +J\}$. The proofs use the stronger result about the containment of *uniform Kuratowskians* into every non-planar lattice. We show that computing the *highest energy* states is NP-complete. Again, we will reduce the problem to that of finding the maximum cut in a 3-regular graph.

The analysis of the $\{-J, 0\}$ interactions model is a simple adaptation of the $\{0, +J\}$ case. The only change is that what is computationally intractable about the partition function is now computing the ground states.

THEOREM 3. *Consider the Ising model with interaction energies $\{0, +J\}$. For every non-planar crystal lattice, computing the highest energy states for its finite sublattices is NP-complete. Therefore, computing the partition function for the finite sublattices is also NP-complete.*

Proof of the Theorem. Let us consider L a non-planar crystal lattice, and let $\mathcal{K}'$ be its Uniform Kuratowskian. Let us assign weight 0 to every edge of L that is not in $\mathcal{K}'$. It is easy to see that computing the highest energy states is equivalent to the computation of the largest cut in the graph. Due to uniform universality of embedding, for every 3-regular graph G, we can find an uniform subdivision G' of G contained in $\mathcal{K}'$. Let us assign weight 0 to every edge that is not in G', and weight $+J$ to every edge in G'. The Lemma 4 shows that computing the maximum cut on these uniformly dialated 3-regular graphs is reducible to computing the maximum cut in 3-regular graphs, and therefore, it is NP-complete. As computing the highest energy states is NP-complete, the partition function is also intractable.

For a positive integer k, the k-dialation of a graph G is a subdivision of the graph in which every edge of G is replaced by a vertex disjoint path of with k new nodes, i.e., having $(k + 1)$ edges.

LEMMA 4. *For every 3-regular graph G, let k be an even number, and let $G^{(k)}$ be the k-dialation subdivision of G. Then G has a cut of size $\geq c$ if and only if $G^{(k)}$ has a cut of size $\geq c + k \mid E(G) \mid$.*

Proof.
Let G be an arbitrary 3-regular graph, and $G^{(k)}$ its k-dialation subdivision.

• Clearly, if G has a cut C with c edges, then $G^{(k)}$ has a cut C' of size $c+k \mid E(G) \mid$. Indeed, every edge e of G is dialated to a path p_e of odd size, because k is even. For each edge of G in C, the edges of the path p_e will alternate in the cut C' crossing from one side to another in the cut. For every edge e of G not in C, with exactly one exception, all the edges of its path p_e, will alternate in the cut C'. Therefore, for every edge e of G, every path p_e contributes with k edges in the cut C', a total of $k \mid E(G) \mid$ edges. For each edge in C, its path contributes with one more edge in C', a total of c more edges.

• Suppose that $G^{(k)}$ has a cut C' of size $c + k \mid E(G) \mid$. Let us consider for every e the path p_e and its structure with respect to the cut. Let A, B be the set of edges e of G for which their p_e is with both endpoints on the same side of the cut, and respectively, with one endpoint in one side, and the other in the other side. Suppose $\mid B \mid < c$. As each edge in A can contribute to at most k edges, and only edges in B can contribute with $k + 1$ edes, we have that the size of the cut C' is $\leq k \mid A \mid + k \mid B \mid + c = k \mid E(G) \mid + c$ which is a contradiction. So $\mid B \mid \geq c$. But each path p_e now can be contracted to the edge connecting its endpoints, such that we have all paths in A giving rise to edges not in the cut, and all paths in B giving rise to edges in the cut. The resulting graph is G and the cut is a legitimate cut of G of size $\geq c$.

5.3 Ising Models with $\{-J, +J\}$ Interactions

The analysis of this case reveals similar intractability results. The constructions are involved and will presented in the final version of the paper.

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