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Combinatorial and topological approach to the 3D Ising model

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Abstract. We extend the planar Pfaffian formalism for the evaluation of the Ising partition function to lattices of high topological genus g. The 3D Ising model on a cubic lattice, where g is proportional to the number of sites, is discussed in detail. The expansion of the partition function is given in terms of 2^{2g} Pfaffians classified by the oriented homology cycles of the lattice, i.e. by its spin structures. Correct counting is guaranteed by a signature term which depends on the topological intersection of the oriented cycles through a simple bilinear formula. The role of a gauge symmetry arising in the above expansion is discussed.

The same formalism can be applied to the counting problem of perfect matchings over general lattices and provides a determinant expansion of the permanent of 0–1 matrices.

1. Introduction

The evaluation of the matching polynomial of a general graph with weighted edges is at the same time a root problem for discrete mathematics, statistical mechanics and mathematical chemistry. Even in its simplest version, the so-called *dimer-covering problem*, in which the sites of a lattices have to be covered by non-overlapping arrangements of dimers, the evaluation of the perfect matching polynomial is a fundamental problem for lattice statistics [1–5]. For planar graphs, e.g. 2D regular lattices, the counting problem is easily reduced via Kasteleyn's lattice orientation theorem to the evaluation of a finite number of Pfaffians [1, 6]. Such a computation requires a number of operations which is polynomial in the number of vertices and is considered to be a tractable problem. For instance, the exact analytical solution of the regular 2D Ising model [7] can be easily obtained by expressing the high-temperature loop counting problem in terms of a dimer-covering generating function over a properly decorated lattice [1, 4, 6, 8, 9]. The periodic nature of Kasteleyn's orientation allows for the evaluation of the associated Pfaffian by diagonalization. Similarly, the Pfaffian method has been used in mathematical chemistry [10] to derive the asymptotic number of dimer coverings for any regular surface lattice. Such a number is strictly related to the efficiency of adsorption processes of dimer molecules over surfaces, or to the degeneracy of double bond arrangements in planar organic lattices (the so-called Kekulé structures).

In the case of non-homogeneous planar lattices, even though the closed-form analytical solution is generally impossible to obtain, the Ising and the dimer problems remain tractable in the algorithmic sense [11].

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The nature of the matching problem changes completely if one considers non-planar graphs or lattices [5]. In discrete mathematics, it is known that the counting problem becomes $\#P$-complete [12] and no exact polynomial algorithm exists for the enumeration of coverings.

In statistical mechanics and mathematical chemistry, the interest in non-planar lattices hinges on the fact that they are equivalent to higher-dimensional lattices. The 3D cubic lattice can be considered as a handlebody 2D lattice of topological genus $g = 1 + N/4$, where N is the number of sites. A non-vanishing ratio g/N for $N \to \infty$ is related to an effective dimension $D > 2$ of the lattice, at least as far as its computational complexity is concerned. No exact solution exists for any non-planar lattice model, the simplest case being two coupled 2D Ising models. Similarly, no exact evaluation of dimer coverings over non-planar lattices is available. Of course, there exist several powerful probabilistic algorithms and approximate theories which provide quite accurate information; however, the issue of understanding the onset of intractability is a basic open one.

In this paper we give an explicit formalism which generalizes Kasteleyn's method to arbitrary non-planar graphs. A first step in this direction was obtained in [13] in which the complete solution for the Ising model on a highly symmetric finite lattice of genus $g = 3$ and $N = 168$ vertices was presented. Here we shall extend such formalism to any lattice and provide a general algorithmic procedure for the 3D cubic lattice. The aim of the paper is to link the combinatorial Pfaffian representation used for planar lattices with the topological features of non-planar lattices. As a result, we find an expansion for the 3D partition function in which the role of spin variables is played by a smaller set of binary topological excitations describing spin structures of the embedding surface of the lattice.

As early as 1963, Kasteleyn [1, 6] noticed that the matching polynomial and the Ising partition function could be written as a weighted sum of 2^{2g} Pfaffians. In particular, since that time it has been shown that each Pfaffian can be associated to an element of the group $(\boldsymbol{Z}_2)^g \times (\boldsymbol{Z}_2)^g$.

In what follows we show that the Ising partition function can be written as $Z = (2\cosh(\beta J))^N \boldsymbol{Z}_0(X)$, where J is the spin–spin interaction energy, $X = \tanh(\beta J)$ is the activity of a bond at inverse temperature β and $\boldsymbol{Z}_0(X)$ is the dimer-covering generating function given as a series of Pfaffians with a topological signature. The final formula we shall prove is

$$\boldsymbol{Z}_0(X) = \frac{1}{2^g} \sum_{\{e_k=0,1\}} (-1)^{\sum_{k=2}^{2g} \sum_{k'=1}^{k-1} I[\omega_k, \omega_{k'}] e_k e_{k'}} \boldsymbol{Pf}\left(\Phi\left(\sum_{k=1}^{2g} e_k \omega_k\right), X\right) \tag{1}$$

where the variables $\{e_k = 0, 1\}$ encode the orientation of the $2g$ elementary homology cycles, $I[\omega_k, \omega_{k'}]$ is the topological intersection matrix of the homology cycles ω_k and Φ represents the orientation of the lattice.

The paper is organized as follows. In section 2 we outline some basic results concerning the combinatorial approaches to the 2D Ising model and briefly review the main steps of the so-called Pfaffian method. In section 3 we give a thorough description of the topology of the 3D cubic lattice, thereby fixing the notation. Section 4 is devoted to the generalization of Kasteleyn's theorem and to the description of the gauge symmetry that such a generalization introduces in the problem. In section 5 we analyse the set of cycles and cocycles in terms of which the partition function will be expressed. The construction of a topological intersection formula which gives the sign of the Pfaffians in the expansion of the partition function is given in section 6. The final constructive procedure is then presented in section 7. Section 8 contains some preliminary results on the Pfaffian expansion, whereas in section 9 we discuss the application of the formalism to the dimer covering and the permanent problems.

Throughout the paper a few numerical results will be given in order to provide some (very preliminary) physical insight. The analysis of the physical consequences of the formalism

together with the discussion of the technicalities involved will form the subject of a forthcoming paper [27].

Independently, in [18] some general results that partially overlap with ours are proposed.

2. Review of combinatorial methods

Despite the fact that the original Onsager solution to the 2D Ising model relied on the algebraic transfer matrix method [7], the combinatorial solutions which have followed provide a more direct geometrical insight into 2D critical phenomena and field theories.

While the transfer matrix method can be defined in any dimension, the combinatorial approaches depend strongly on the topology of the space where the lattice is immersed. Very schematically, in two dimensions the sum over spin configurations is recast as a sum over closed curves (loops). Such curves are endowed with both an intrinsic topology and with the extrinsic one of $\mathbb{R}^2$. Since the Ising action depends only on the extrinsic geometry of loops, one has to avoid double counting and a proper cancellation mechanism, a topological term has to be introduced in the sum. Such an approach has been developed by Kac and Ward [14] and probably provides the most natural way of taking the continuum limit toward a field theoretical analysis [15, 16].

In three dimensions, the generalization of the above method encounters enormous difficulties due to the variety of intrinsic surface topologies immersed in 3D lattices. Despite the in-depth work performed attempting to recast the critical 3D Ising problem as a string theory [17], the problem remains unsolved with respect to many aspects.

Here we generalize the 2D (planar) Pfaffian or dimer-covering approach to the Ising model, a purely combinatorial and basic tool of discrete mathematics that has many applications in counting problems [5]. In two dimensions, this approach relies on the equivalence between loop counting and dimer coverings (also referred to as *perfect matchings*) over a suitably decorated lattice. Once such a relationship is established the Pfaffian method turns out to be simple both for the derivation of exact solutions (in the cases of periodic lattices) and for the definition of polynomial algorithms on 2D heterogeneous models [4, 11].

Let us briefly remind ourselves how the method works in the 2D case. The interaction energy of the Ising model on a planar square lattice Λ_{2D} is given by

$$H = -J_1 \sum_{j=1}^{N_1} \sum_{k=1}^{N_2} \sigma_{j,k}\sigma_{j,k+1} - J_2 \sum_{j=1}^{N_1} \sum_{k=1}^{N_2} \sigma_{j+1,k}\sigma_{j,k} \tag{2}$$

where N_1, N_2 are the number of sites in the two orthogonal directions, J_1, J_2 are the spin–spin interaction energies and $\sigma_{j,k} = \pm 1$. The partition function $Z = \sum_{\{\sigma=\pm1\}} \exp(-\beta H)$ can be written as

$$\begin{aligned} Z = (\cosh(\beta J_1)\cosh(\beta J_2))^{N_1 N_2} \sum_{\{\sigma=\pm1\}} \left[\prod_{j=1}^{N_1} \prod_{k=1}^{N_2} (1 + X_1 \sigma_{j,k}\sigma_{j,k+1}) \right] \\ \times \left[\prod_{j=1}^{N_1} \prod_{k=1}^{N_2} (1 + X_2 \sigma_{j,k}\sigma_{j,k+1}) \right] \end{aligned} \tag{3}$$

where $X_i = \tanh(\beta J_i)$ are called the bond activities. Expanding the product and evaluating the sum over $\{\sigma = \pm 1\}$, all the terms containing odd powers of σ give no contribution, whereas all even powers may be replaced by 1. It follows that the partition function acquires a clear interpretation as generating functions of closed loops with p horizontal and q vertical bonds

with no overlapping sides. In fact, denoting with N_{pq} the number of such loops, we have

$$Z = (2\cosh(\beta J_1)\cosh(\beta J_2))^{N_1 N_2} \sum_{p,q} N_{pq} X_1^p X_2^q. \tag{4}$$

In turn, the above expansion can be mapped onto the problem of evaluating the generating function of dimer coverings (the so-called weighted matching polynomial) over a new 'counting' lattice $\Lambda_{2D}^{\#}$ obtained by substituting each site of the original lattice with a cluster of six sites (two triangles with a joining bond) and by assigning activity 1 to the new decorating bonds while retaining the activity of the bonds inherited by the original lattice. The (eight) possible configurations of loop bonds at any Ising site are in one-to-one correspondence with perfect dimer configurations on the decorating cluster. Therefore, the sum in (4) coincides with the generating functions of perfect matchings over the decorated lattice.

Finally, in order to compute Z we orient the lattice according to the Kasteleyn prescription by assigning arrows to each bond in such a way that for any closed circuit ℓ on $\Lambda_{2D}^{\#}$, the number of bonds of ℓ oriented clockwise is of opposite parity to the number of sites enclosed by ℓ. The Kasteleyn rules define completely the orientation for planar lattices, whereas for non-planar lattices, i.e. lattices which can be immersed on surfaces of non-trivial topological genus, we need further sign fixing for loops not homologically trivial (i.e. without an interior). The dimer-covering generating function can then be expressed as a weighted sum of Pfaffians of the antisymmetric adjacency matrix with elements given by the activities of the bonds and signs determined by their orientation. By virtue of the Cayley theorem, Pfaffians are computed as square roots of the determinant of such matrices. Thus, the Ising partition function can be written explicitly as a determinant which for uniform interaction energies can be further block diagonalized by Fourier transform. The final calculation of a 6×6 determinant leads to the exact closed form expression of the 2D Ising partition function. A thorough discussion of the above procedure can be found in [4].

Below we shall concentrate on the generalization of the above construction to the cubic 3D lattice. The procedure is, however, general and can be straightforwardly generalized to any non-planar lattice. A first explicit example was presented in [13] for the case of group lattices with non-trivial topological genus. The same inductive reasoning used in [13] leads to a simple topological expression for the coefficients in the Pfaffian expansion.

3. The 3D cubic lattice and embedding surface

We consider 3D cubic lattices Λ of sides N_1, N_2, N_3, with $N = N_1 N_2 N_3$ sites and periodic boundary conditions. Each vertex V is identified by a triple of periodic coordinates $\{n_1, n_2, n_3\}$, $n_i = 0, \ldots, N_i - 1$, with $V(n_1, n_2, n_3) \equiv V(\mathrm{mod}(n_1, N_1), \mathrm{mod}(n_2, N_2), \mathrm{mod}(n_3, N_3))$. The sites can also be labelled in sequential order by the single index $q \equiv q(n_1, n_2, n_3) = \mathrm{mod}(n_1, N_1) + N_1 \mathrm{mod}(n_2, N_2) + N_1 N_2 \mathrm{mod}(n_3, N_3)$ with the inverse relations, $n_1 = \mathrm{mod}(q, N_1)$, $n_2 = \mathrm{mod}(\frac{q-n_1}{N_1}, N_2)$ and $n_3 = \mathrm{mod}(\frac{q-n_1-n_2 N_1}{N_1 N_2}, N_3)$. In what follows notations and operations over the integers n_1, n_2, n_3 have to be understood modulo N_1, N_2, N_3, respectively.

The lattice Λ is invariant under translations $D_i : n_i \to n_i + 1$.

The set of $N_b = 3N$ bonds $L_i(q)$, $i = 1, 2, 3$ of Λ connects couples of neighbouring sites $\{V(q), V(D_i q)\}$, thus defining the adjacency or incidence matrix A of Λ, $A_{q,q'} = 1$ if q and q' are connected by a bond and $A_{q,q'} = 0$ otherwise.

We call *plaquette* a square face $F_{i_1}(n_1, n_2, n_3) \equiv F_{i_1}(q)$ of Λ identified by the sequence of vertices, $V(q)$, $V(D_{i_2} q)$, $V(D_{i_2} D_{i_3} q)$, $V(D_{i_3} q)$, where with the notation i_1, i_2, i_3 we denote a generic cyclic permutation of the indices 1, 2, 3. Λ contains three classes of N plaquettes

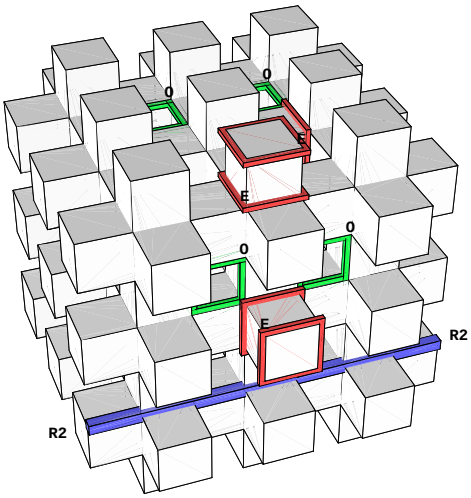

Figure 1. Orientable surface Σ of genus $g = N/4 + 1$ containing all sites and bonds of the 3D cubic lattice Λ. Some examples of the even (E), odd (O) and exceptional (R) cycles are also shown.

$F_i(q)$, orthogonal to the axes i, $(i = 1, 2, 3)$.

The parity of a site is given by $p(q) = (-1)^{n_1+n_2+n_3}$. Λ is a bipartite lattice in that edges always connect vertices of opposite parity.

In order to implement the dimer method we construct an orientable surface Σ without boundary, which contains all the sites and bonds of Λ and is the union of a subset of square plaquettes of Λ. The number N_f of such plaquettes is $N_f = N_b/2 = 3N/2$, each bond belonging to two plaquettes of the surface and each plaquette containing four bonds. It follows that N and at least one of the numbers N_1, N_2, N_3 need to be even. For simplicity we shall assume $N_i = 2M_i$, so that $N = 8M$ with $M = M_1M_2M_3$.

As we shall see, all the above conditions can be matched by a definition of Σ which preserves part of the symmetries of the original lattice.

The topological genus g of the surface, evaluated by Euler's formula, is $N - N_b + N_f = 2(1 - g)$, from which it follows $g = 1 + 2M = 1 + N/4$.

The definition of Σ requires that a plaquette $F_{i_1}(q)$ belongs to Σ only if $n_{i_2} + n_{i_3}$ is odd, and we shall call such plaquettes *faces*. The final result for Σ consists of a square-beam periodic structure as shown in figure 1.

3.1. Combinatorial topology of the 3D cubic lattice

In order to proceed in the generalization of the Pfaffian method it is useful to recall some basic notions of combinatorial topology [20].

Sites, bonds and faces of Σ generate Abelian groups, additive modulo 2, of non-oriented chains $C_k(\Sigma, \boldsymbol{Z_2})$ of dimension $k = 0, 1, 2$, respectively. For any $c \in C_k(\Sigma, \boldsymbol{Z_2})$, we have $c + c = 0$, where 0 is the identity of the group.

The linear boundary operator δ maps chains of different dimensions $\delta : C_k(\Sigma, \boldsymbol{Z_2}) \to C_{k-1}(\Sigma, \boldsymbol{Z_2})$ and is defined as follows:

$$\begin{aligned} &\delta V(q) = 1 \\ &\delta L_i(q) = V(q) + V(D_i q) \\ &\delta F_{i_1}(q) = L_{i_2}(q) + L_{i_3}(D_{i_2} q) + L_{i_2}(D_{i_3} q) + L_{i_3}(q). \end{aligned} \tag{5}$$

Clearly, $\delta^2 = 0$. A chain c_k in the kernel of δ, i.e. such that $\delta c_k = 0$, is said to be closed. A *circuit* is a closed sequence of vertices connected by edges, where each edge is an element of

$C_1(\Sigma, \boldsymbol{Z_2})$, the sum of edges of a circuit is a closed 1-chain c_1.

A chain $c_{k-1} = \delta c_k \in C_k(\Sigma, \boldsymbol{Z_2})$ is called a *boundary*. Since $\delta^2 = 0$, a boundary c_1 is necessarily closed and reduces to a sum of circuits.

We will also keep the definition of $\delta F_i(q)$ as given by (5) in the improper case in which $F_i(q)$ is not a face, and hence $\delta F_i(q)$ is not a boundary but only a circuit on Σ.

Boundaries and closed chains of $C_k(\Sigma, \boldsymbol{Z_2})$ generate the subgroups $B_k(\Sigma, \boldsymbol{Z_2}) \subset Z_k(\Sigma, \boldsymbol{Z_2}) \subset C_k(\Sigma, \boldsymbol{Z_2})$, respectively.

The homology group is thus defined by $H_k(\Sigma, \boldsymbol{Z_2}) = Z_k(\Sigma, \boldsymbol{Z_2})/B_k(\Sigma, \boldsymbol{Z_2})$ so that there exists a projection π from closed chains to the elements of H_1, $\pi : Z_1(\Sigma, \boldsymbol{Z_2}) \to H_1(\Sigma, \boldsymbol{Z_2})$. Boundaries are topologically trivial since they are mapped by π onto the identity 0 of the homology groups. The elements of $H_1(\Sigma, \boldsymbol{Z_2})$ are called cycles and the homology group is generated by a base of $2g$ elementary cycles which are equivalence classes of closed chains under the addition of boundaries. A closed chain $c_k \in Z_k(\Sigma, \boldsymbol{Z_2})$ such that $\pi c_k = \gamma_k \in H_k(\Sigma, \boldsymbol{Z_2})$, is called a representative of γ_k.

The multiplicative functionals on the elements of $C_k(\Sigma, \boldsymbol{Z_2})$ and $H_k(\Sigma, \boldsymbol{Z_2})$ with values ± 1 constitute groups of cochains and cocycles denoted by $C^k(\Sigma, \boldsymbol{Z_2})$ and $H^k(\Sigma, \boldsymbol{Z_2})$, respectively. The definitions of $H_k(\Sigma, \boldsymbol{Z_2})$ and $H^k(\Sigma, \boldsymbol{Z_2})$ are independent from the triangulation of the surface Σ and, in particular, will be valid for the decorated lattice Γ defined in the following section. The properties of the groups $H_k(\Sigma, \boldsymbol{Z_2})$ and $H^k(\Sigma, \boldsymbol{Z_2})$ depend only on the topological features of Σ and not on the choice of the tessellating lattice.

The symmetry properties of Σ can be seen more clearly by considering its embedding into the subset or box Ξ of $\mathbb{R}^3$ defined by $0 \leqslant x < N_1$, $0 \leqslant y < N_2$, $0 \leqslant z < N_3$ with periodic boundary conditions. The complement $\Xi - \Sigma$ is the union of two open and disjoint subsets Ξ_+, Ξ_- congruent under the translation $S = D_1 D_2 D_3$ and invariant under $T_i = D_i^2$. S and $\{T_i\}$ generate the symmetry group of Σ while D_i alone is not a symmetry of Σ. The closure of Ξ_+, Ξ_- is given by $\Xi^+ = \Xi_+ \cup \Sigma$, $\Xi^- = \Xi_- \cup \Sigma$ and $\Xi^+ \cap \Xi^- = \Sigma$. We may conventionally regard Ξ^+ as the interior of Σ. On Ξ^+, the bond $L_i(q)$ is convex/concave depending on whether $n_i(q)$ is odd/even, hence, moving along Ξ^+ with D_i, we encounter alternatively convex and concave bonds. On Ξ^+, each face has two concave and two convex bonds which interchange if we focus on Ξ^- rather than Ξ^+.

4. Kasteleyn's orientation and gauge symmetry

4.1. Decorated counting lattice

In order to write the Ising partition function as a dimer-covering generating function we first construct a decoration Γ of Σ obtained, following Fisher's prescription [8], by replacing each site of coordination q with a graph of $3(q-2)$ points and $q-2$ triangular faces, as shown in figure 2 (for the case of interest here $q = 6$). In our case, the decorated surface Γ contains $12N$ vertices.

Each face of Σ maps into a face of Γ composed of four bonds inherited from Σ plus eight bonds introduced by the decoration. Each site of Σ originates four triangular faces in Γ, see figure 2(*b*). As we shall see, the above decoration is also equivalent (with respect to dimer-covering configurations) to a locally non-planar one in which each site of Σ yields a complete graph of six vertices, see figure 2(*c*).

Clearly, the homology groups of Γ and Σ coincide and will be identified.

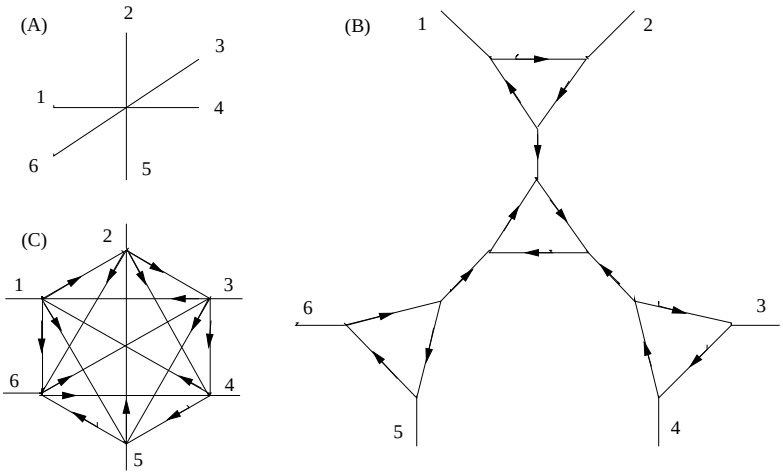

Figure 2. Oriented decorating clusters. Each site (*a*) is replaced by either Fisher's planar decoration (*b*) or the equivalent complete graph (*c*).

4.2. Proper orientations

The orientation over bonds is an additional geometrical structure Φ defined by a function $\phi_j(q) = \pm 1$, $j = -3, -2, -1, 1, 2, 3$, such that $\phi_j(q) = 1$ (resp. -1) corresponds to a bond oriented from $V(q)$ to $V(D_j q)$ (resp. from $V(D_j q)$ to $V(q)$), and $\phi_{-j}(q) = -D_j^{-1}\phi_j(q)$.

An orientation of the bonds of Γ or Σ is said to be *proper* if it satisfies the condition of Kasteleyn's theorem for planar lattices, i.e. if by moving anticlockwise along the perimeter of a face we encounter an odd number of oppositely oriented bonds. Unless otherwise specified we assume in the following that all orientations Φ are proper. Consider now a boundary on Γ or Σ consisting of a single circuit and containing k points in the interior. By induction it follows that moving along it anticlockwise we encounter a number of oppositely oriented bonds with parity opposite to that of k. A proper orientation of Σ defines a proper one for Γ as follows. Bonds of Γ inherited from Σ are given the same $\phi_j(q)$. Bonds forming the boundary of an ornating triangle are then all clockwise oriented so they appear anticlockwise in the adjacent faces of Γ inherited from Σ and lead to a proper orientation. Sites of Σ and corresponding decorating clusters of Γ fall into two subsets of even and odd sites according to their parity $p(q)$.

4.3. Gauge group

Given a proper orientation Φ of Γ, it is possible to derive different but equivalent ones by reversing all the bonds of Γ which are incident to a given site $V(q)$, according to the local *gauge* operation (see figure 3)

$$g(q) : \phi_j(q) \to -\phi_j(q) \qquad \forall j. \tag{6}$$

The operations $\{g(q)\}$ generate the *gauge* group $\mathcal{G}$. The orientations generated by $\mathcal{G}$ are equivalent and will be identified. By using $\mathcal{G}$ we can fix arrows on Γ such that they relate even and odd clusters by a mirror reflection and reversal of orientations of all the bonds.

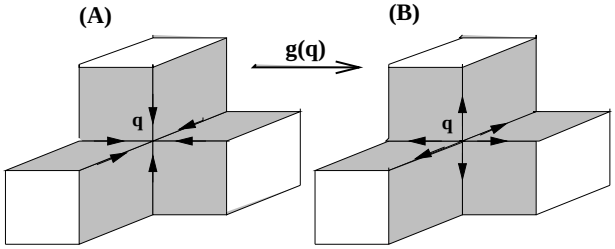

Figure 3. Elementary *gauge* operation. The orientation parity of the faces remains unaltered.

4.4. Generalized Kasteleyn rule for dimer coverings

A dimer covering of Γ is defined by a two-colouring (say black or white) assignment to the edges of Γ such that each site of Γ belongs exactly to one black bond. By superposing two dimer coverings we obtain a set of closed black circuits which cover all vertices of Γ. By moving around a circuit we encounter an alternating sequence of black bonds from each of the two coverings, therefore the length of the circuit must be even. If the circuit is a boundary it must enclose points which are themselves connected by bonds forming black circuits, thus the number of points inside must also be even and by moving around the circuit in whatever direction we encounter an odd number of opposite arrows.

Dimer configurations are in one-to-one correspondence with terms of the Pfaffian of an antisymmetric incidence matrix $M(\Phi, X)$ which will be uniquely defined further on by the pair (Γ, Φ). In what follows we shall use one-chains composed of black circuits only, originating from the superposition of dimer coverings. For simplicity, since no confusion will arise, we use for the black subgroups and the corresponding dual groups the same notation $B_1(\Sigma, \boldsymbol{Z_2})$, $Z_1(\Sigma, \boldsymbol{Z_2})$ and $H_1(\Sigma, \boldsymbol{Z_2}) = Z_1(\Sigma, \boldsymbol{Z_2})/B_1(\Sigma, \boldsymbol{Z_2})$ introduced in the previous section for the full groups.

Adding a boundary to a black circuit c does not alter its orientation. The latter depends, therefore, only on the image $\gamma = \pi(c) \in H_1(\Sigma, \boldsymbol{Z_2})$ and defines a functional $\Phi(c)$. From the bond orientation function $\phi_i(q)$ we define the orientation function $\Phi_{i_1}(q)$ for the boundary of the faces $\delta F_{i_1}(q)$ as the multiplicative and gauge-invariant functional

$$\Phi_{i_1}(q) = -\phi_{i_2}(q)\phi_{i_3}(D_{i_2}q)\phi_{-i_2}(D_{i_2}D_{i_3}q)\phi_{-i_3}(D_{i_3}q). \tag{7}$$

For a black boundary, Kasteleyn's rule implies

$$\Phi_i(q) = 1 \qquad i = 1, \ldots, 3 \qquad q = 1, \ldots, N. \tag{8}$$

Given an anticlockwise sequence of bonds $L_{k_j}(q_j)$ forming the circuit $c_1 \in C_1(\Sigma, \boldsymbol{Z_2})$ and connecting the points $V(q_j)$, $j = 1, \ldots, m$, the orientation $\Phi(c_1)$ over $H_1(\Sigma, \boldsymbol{Z_2})$ is defined by

$$\Phi(c_1) = -\Pi_{j=1}^{m}\phi_{k_j}(q_j). \tag{9}$$

On a lattice of non-trivial genus g ($g > 0$) such a functional is not an element of $H^1(\Sigma, \boldsymbol{Z_2})$, i.e. in general $\Phi(c_1 + c_2) \neq \Phi(c_1)\Phi(c_2)$, as it can be readily verified in the simple 2D Ising lattice with periodic boundary conditions but also on other finite lattices [13]. The argument runs as follows.

The single black circuit $c_{1,2}$ given by the sum $c_1 + c_2$ of two black circuits c_1 and c_2 of parity $\Phi(c_1)$ and $\Phi(c_2)$ respectively, which intersect p times, has parity

$$\Phi(c_{1,2}) = (-1)^p\Phi(c_1)\Phi(c_2). \tag{10}$$

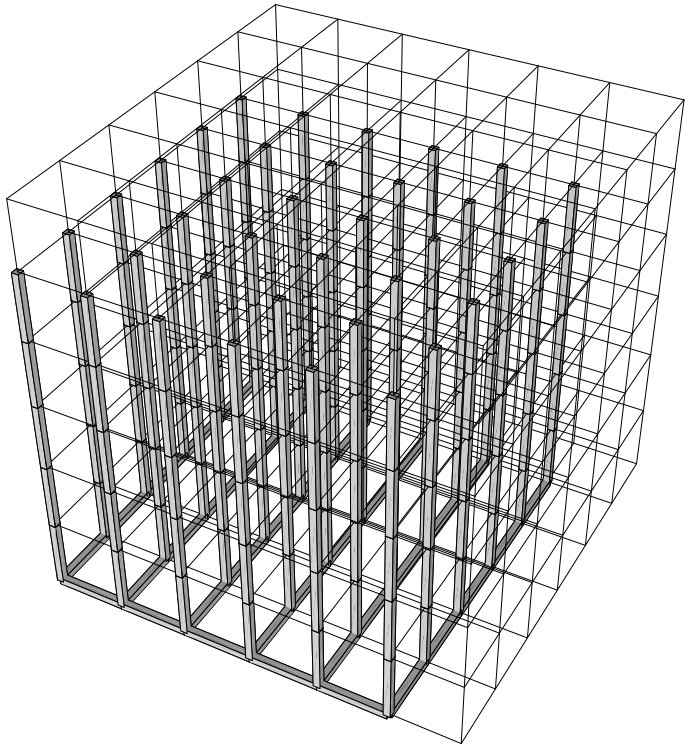

Figure 4. 3D simple cubic lattice and the axial gauge tree $\mathcal{T}$.

This fact will turn out to be essential in determining the signs with which the Pfaffians have to appear in the expansion of the generating function. Let us consider the specific example of the sum of two black circuits c_1 and c_2 of parity $\Phi(c_1)$ and $\Phi(c_2)$ with representatives $a + \ell$ for c_1, $b + \ell$ for c_2, where ℓ is a common bond and a, b are paths closed by ℓ. A representative for the product c_{12} is now $a + b$.

We move along c_1 in a specific direction encountering n_a opposite arrows along a and $r = 0, 1$ opposite arrow coming from ℓ with a total of $n_a + r$. Similarly, we proceed along c_2 in such a way that when we move along $c_{1,2}$, a and b run in the same direction and meet a number $n_b + 1 - r$ of opposite arrows since ℓ is run in the opposite direction in c_2 with respect to c_1. The total number of opposite arrows along $c_{1,2}$ is now $n_a + n_b$ while the total on c_1, c_2 is $n_a + n_b + 1$. This result is equivalent to (10) for $p = 1$ and can be generalized to multiple intersections.

4.5. Gauge tree, spin structures and Pfaffian matrices

The gauge symmetry G can be used to fix the orientation on a subset of bonds forming a spanning tree $\mathcal{T}$ in Γ, see figure 4. It will be seen that both the gauge choice and Kasteleyn's rules lead to a number of orientations which is 2^{2g}. Such orientations break all symmetries of Σ and are in one-to-one correspondence with the 2^{2g} spin structures of a surface of genus g.

For each element of the base of $H_1(\Sigma, \boldsymbol{Z_2})$ there exist two possible orientations, for a total of 2^{2g} different global orientations of Σ. Given Φ for the cycles of the homology base, it is possible to derive the parity of any circuit by the intersection formalism related to (10).

Φ defines (modulo gauge transformations) an antisymmetric matrix $M(\Phi, X)$ of dimension $12N \times 12N$ with elements labelled by the sites of Γ. Changing the gauge produces a new matrix $M'(\Phi, X) = KM(\Phi, X)K^{-1}$, with K diagonal, which has the same Pfaffian of $M(\Phi)$.

If q, q' are not connected we set $M_{q,q'}(\Phi, X) = 0$. If q, q' are connected by a decorating bond $L_i(q)$, we have $M_{q,q'}(\Phi, X) = \phi_i(q) = \pm 1$ depending on the orientation of the bond. If q, q' are connected by a bond inherited from Λ, we set $M_{q,q'}(\Phi, X) = \phi_i(q)X = \pm X$, where X is the so-called activity of the bond, $X = \tanh(\beta J)$, where β is the inverse temperature and J the spin interaction energy. The diagonal 12×12 blocks of $M(\Phi, X)$ describe the decorating clusters displayed in figure 2(*b*) and are given by

$$\begin{vmatrix}
0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
-1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 1 & -1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & -1 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 & -1 & 0
\end{vmatrix} \tag{11}$$

We have thus defined all the elements of $M(\Phi, X)$ which can be written as

$$M(\Phi, X) = A + XB(\Phi) \tag{12}$$

where A is block diagonal consisting of $N/2$ fixed blocks as in (11), corresponding to even sites and $N/2$ opposite blocks corresponding to odd sites. $B(\Phi)$ contains $\phi_i(q)$. For computational purposes the matrix $M(\Phi, X)$ can be replaced by an equivalent one of dimensions $12M \times 12M$ by a folding procedure which we can sketch as follows. In this section $\boldsymbol{I}_n$ denotes the identity matrix of rank n.

(i) The $12N$ sites are grouped into two subsets each of $6N$ sites. The first subset, Ext, includes the internal sites of each of the N decorating clusters, which in (11) label rows and columns $6, \ldots, 12$. Each of these rows and columns have three non-zero entries. The second subset Int contains sites with two decorating bonds (the two non-zero entries in (11)) and one inherited from Σ which appears in B. Schematically, $M(\Phi, X)$ can be written in blocks M_{ik} of the form

$$M(\Phi, X) = \begin{vmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{vmatrix} \tag{13}$$

where $i, k = 1, 2$ label the subsets Ext, Int respectively. But now M_{11} is a block diagonal matrix with $\mathrm{Det}(\mathrm{M}_{11}) = 1$ and which can be easily inverted. We then write

$$\det(M) = \det(M_{11}) \det(M_{22} - M_{21}M_{11}^{-1}M_{12}) = \det(M_a). \tag{14}$$

$M_a = M_{22} - M_{21}M_{11}^{-1}M_{12}$ is now a $6N \times 6N$ matrix where the decoration now reduces to complete graphs of order 6 shown in figure 2(*c*).

(ii) The $6N$ Ext entries in M_a are again partitioned into two subsets labelling even and odd sites respectively, thus exploiting the fact that Σ is a bipartite graph. Schematically, M_a can be written as

$$M_a = \begin{vmatrix} M_{EE} & M_{EO} \\ M_{OE} & M_{OO} \end{vmatrix}. \tag{15}$$

Now M_{EE}, M_{OO} do not contain X since an inherited bond always connects sites of opposite parity, while M_{EO}, M_{OE} are instead linear in X. We may again apply (14) and obtain a $3N \times 3N$ matrix of the form

$$M_b(\Phi, X^2) = A_b + X^2 B_b(\Phi) \tag{16}$$

such that $\det(M_a) = \det(M_b)$.

It can be verified that the diagonal matrix $\Omega = \boldsymbol{I}_N \otimes \mathrm{Diag}(1, 1, 1, -1, -1, -1)$ obeys the relations

$$\Omega A_c \Omega = A_b^{-1} \qquad \Omega B_c \Omega = B_b^{-1} \tag{17}$$

and that A_b, B_b share the same spectrum with eigenvalues $\pm\mathrm{i}$, $\pm\mathrm{i}(2 - \sqrt{3})$, $\pm\mathrm{i}(2 + \sqrt{3})$ independently of Φ and $\det A_b = \det \Omega = 1$. The essential information is now contained in B_b and X since A_b is a fixed numerical matrix.

By Cayley's theorem the determinant of $M(\Phi, X)$ or $M_b(\Phi, X^2)$ is the square of an even polynomial $\boldsymbol{Pf}(\Phi, X)$ in the activity X called the Pfaffian of $M(\Phi, X)$.

As we shall see, the ambiguity of sign in the extraction of the square root can be solved by imposing all Pfaffians to be $= 1$ in the high-temperature limit $X \to 0$. However, the polynomial $\boldsymbol{Pf}(\Phi, X)$ may have zeros on the real axis in the physical range $X = 0, 1$ and may change sign when reaching $X = 1$. By generalizing the results of [13] we find that the sign in $X = 1$ is given by the function $\sigma(\boldsymbol{a})$ defined below in (43), having a precise topological meaning.

(iii) We have:

$$\det M_b(\Phi, X^2) = \det(A_b + X^2 B_b) = \det(\boldsymbol{I}_{3N} + X^2 A_b^{-1} B_b) = \det(\boldsymbol{I}_{3N} + X^2 U_b) \tag{18}$$

where $U_b = A_b^{-1} B_b$.

Let $\Theta = \Omega A_b$, so that $\Theta^2 = \boldsymbol{I}_{3N}$ and

$$\Theta U_b \Theta = \Theta A_b^{-1} B_b \Theta = \Omega B_b \Omega A_b = B_b^{-1} A_b = U_b^{-1} \tag{19}$$

where Θ is once again a block 6×6 matrix which can be explicitly diagonalized so that by changing basis both Θ and U can be written in the following block form where briefly $\boldsymbol{I} = \boldsymbol{I}_{12M} = \boldsymbol{I}_{3N/2}$:

$$\Theta = \begin{vmatrix} \boldsymbol{I} & 0 \\ 0 & -\boldsymbol{I} \end{vmatrix} \qquad U_b = \begin{vmatrix} Q & R \\ S & T \end{vmatrix}. \tag{20}$$

From (19) we see that Q, R, S, T satisfy the identities

$$Q^2 - RS = \boldsymbol{I} \qquad Q = RTR^{-1} \qquad Q = S^{-1}TS. \tag{21}$$

We have now

$$\begin{aligned} \det(\boldsymbol{I} + X^2 U_b) &= \det \begin{vmatrix} \boldsymbol{I} + X^2 Q & X^2 R \\ X^2 S & \boldsymbol{I} + X^2 T \end{vmatrix} \\ &= \det \left(\begin{vmatrix} \boldsymbol{I} & 0 \\ 0 & S \end{vmatrix} \begin{vmatrix} \boldsymbol{I} + X^2 Q & X^2 RS \\ X^2 & \boldsymbol{I} + X^2 S^{-1} T S \end{vmatrix} \begin{vmatrix} \boldsymbol{I} & 0 \\ 0 & S^{-1} \end{vmatrix} \right) \end{aligned} \tag{22}$$

but now S can be included in the changes of basis and we can assume $S = 1$, $T = Q$, $R = Q^2 - \boldsymbol{I}$. Therefore, we may simply write

$$\begin{aligned} \det(\boldsymbol{I} + X^2 U_b) &= \det \begin{vmatrix} \boldsymbol{I} + X^2 Q & X^2(Q^2 - 1) \\ X^2 & \boldsymbol{I} + X^2 Q \end{vmatrix} = \det \begin{vmatrix} 0 & -(X^4 + 1)\boldsymbol{I} - 2X^2 Q \\ \boldsymbol{I} & \boldsymbol{I} + X^2 Q \end{vmatrix} \\ &= \det((X^4 + 1)\boldsymbol{I} + 2X^2 Q) = X^{24M} \det((X^2 + X^{-2})\boldsymbol{I} + 2Q) \end{aligned} \tag{23}$$

where we subtracted from the upper block row the lower block row multiplied by $Q + X^{-2}$. In the last form the determinant is evaluated for a matrix $(X^4 + 1)\boldsymbol{I} + 2X^2 Q$ of rank $12M$, a factor 8 down from $M(\Phi, X)$, with a considerable gain in computational speed. Clearly, $\boldsymbol{Pf}(\Phi, X) X^{-12M}$ is invariant under the map $X \to X^{-1}$.

5. Cycles and cocycles over Σ

The black elements of $H_1(\Sigma, \boldsymbol{Z_2})$ are generated by two classes of elementary cycles $E_{i_1}(q)$, $O_{i_1}(q)$, referred to as even or odd cycles forming the sets E, O. Such cycles are homologically equivalent over Γ to cycles of the form

$$L_{i_2} + L_{i_3}(D_{i_2}q) + L_{i_2}(D_{i_3}q) + L_{i_3}(q) \tag{24}$$

where n_{i_1}, n_{i_2} are even/odd for cycles $\in E/O$.

Cycles $\in \{E, O\}$ are thus generated by the boundaries $\delta F_i(q)$ of the $12M = 3N/2$ plaquettes of Γ which are not faces of Σ (see figure 1).

However, these cycles are not independent since their number is $6M > 2(1 + 2M) = 2g$. In order to perform a correct counting we consider the following product of six plaquettes for $n_1 + 1, n_2, n_3$ even (remember that $q \equiv (n_1, n_2, n_3)$):

$$E_1(D_1q) + E_1(q) + \delta F_2(q) + \delta F_2(D_2q) + \delta F_3(q) + \delta F_3(D_3q) \tag{25}$$

i.e. the boundaries of the plaquettes of the elementary cube $C(q)$ obtained by translating of the site $V(q)$ by one unit along the positive direction of all three axes. By expanding the product (25) each bond appears twice, whence follows the equivalence modulo a boundary of $E_1(D_1q)$ and $E_1(q)$, which are identified in E. Indeed the parity of the last four plaquettes indicates that they must be faces of Σ and are topologically trivial. Both in $F_3(n_1, n_2, n_3)$, $F_3(n_1, n_2, n_3 + 1)$ the sum $n_1 + n_2$ is odd, while in $F_2(n_1, n_2, n_3)$, $F_2(n_1, n_2 + 1, n_3)$ the sum $n_1 + n_3$ is odd. It follows that they have boundaries equivalent to the identity of $H_1(\Sigma, \boldsymbol{Z_2})$ and that

$$\begin{aligned} &E_i(D_iq) = E_i(q) \qquad n_i \text{ odd} \\ &O_i(D_iq) = O_i(q) \qquad n_i \text{ even.} \end{aligned} \tag{26}$$

Each cube of Λ gives an identity among cycles, but their actual role depends on the parity of n_1, n_2, n_3.

If n_1, n_2, n_3 all have the same parity, the boundary of the cube does not contain faces and leads to the identity

$$\sum_{i=1}^{3}(E_i(q) + E_i(D_iq)) = 0 \tag{27}$$

which connects six cycles of the same parity and must be added to the previous identities. We shall denote with $\mathcal{E}$ and $\mathcal{O}$ the set of values of q restricted to n_1, n_2, n_3 all even and all odd, respectively. If $q \in \mathcal{E}$, the cubes $C(q)$ and $C(T_iq)$ are continuous and contain the common cycle $E_i(D_iq) = E_1(T_iq)$. It follows that the M identities deriving from the even cubes are not independent because in their sum each cycle appears twice. The same reasoning applies to the odd cubes. Thus we may write

$$\sum_{q\in\mathcal{E}} E_i(q) = 0 \qquad \sum_{q\in\mathcal{O}} O_i(q) = 0. \tag{28}$$

Another class of identities connects even with odd cycles. Consider the plane of Λ with n_3 constant. Such a plane is tessellated by plaquettes which are faces if $n_1 + n_2$ is odd and otherwise have boundaries (on Λ but not on Σ) which are cycles $\in E_3(q)$ or $O_3(q)$. By virtue of the periodicity of Λ the plane has toroidal topology and the sum of the boundaries of all the plaquettes is 0. We thus have the identities

$$e(n_3) = \sum_{n_1,n_2 \text{ even}} E_3(n_1, n_2, n_3) = o(n_3) = \sum_{n_1,n_2 \text{ odd}} O_3(n_1, n_2, n_3). \tag{29}$$

Replacing n_3 with $n_3 - 1$ in the above expressions we obtain the same identity due to (26).

Such a result can be further extended as follows. If n_3 is even, we have $e(n_3) = e(n_3 - 1)$. Let us consider the product of the boundaries of the cubes $C(n_1, n_2, n_3)$ where n_3 is a fixed even index and n_1, n_2 are even

$$\sum_{n_1,n_2 \text{ even}, i=1,2,3} [E_i(n_1, n_2, n_3) + E_i(D_i(n_1, n_2, n_3))]. \tag{30}$$

Factors of the type $E_1(n_1, n_2, n_3)$, $E_2(n_1, n_2, n_3)$ always appear twice in contiguous cubes, and the products can be written as

$$\sum_{n_1,n_2 \text{ even}} [E_3(n_1, n_2, n_3) + E_3(n_1, n_2, n_3 + 1)] = e(n_3)e(n_3 + 1) \tag{31}$$

from which we have $e(n_3) = e(n_3 + 1)$. It follows that $e(n_3)$ does not depend on n_3. The same result holds for all directions and for cycles of odd arguments. Form (29) we have $e(n_i) = o(n_i) \equiv I_i$, providing three exceptional identities $I_i (i = 1, \ldots, 3)$, which connect cycles of different parity.

Finally, we have three exceptional cycles $R_i(q) (i = 1, \ldots, 3)$ given by

$$R_i(q) = \sum_{n=0,1,\ldots,N_i-1} L_i(D_i^n q). \tag{32}$$

We set $R_i = R_i(0)$. Each $R_i(q)$ can be expressed in terms of R_i and of E, O cycles. Note that $R_i(q)$ does not depend on n_i and hence can be written in terms of two site labels and a direction, e.g. $R_1(q) = R_1(n_2, n_3)$. Geometrically, $R_1(q)$ is a straight circuit which winds around Λ by exploiting the periodicity, its length is $N_1 = 2M_1$ and is even (see figure 1). There is no ambiguity in extending formula (9) to black $R_i(q)$. The existence of $R_i(q)$ follows from the periodicity conditions imposed on Λ and also exists in the 2D Ising model where they produce the analogue of $R_i(q)$ for $i = 1, 2$. There is, however, no 2D analogue of the E, O cycles.

We are now in position to check that the overall number of independent cycles is in fact $2g$. To each one of the M even/odd cubes corresponds one identity but only $M - 1$ of them are independent. The $3M$ even/odd cycles we started with reduce to $3M - (M - 1) = 2M + 1 = g$ independent ones, giving an exact overall number of $2g$. The three cycles that are eliminated by the identities I_i are replaced by the exceptional cycles R_i so that the overall counting remains unaltered. (In the thermodynamic limit $N \to \infty$, we expect a negligible contribution from the surface terms R_i.)

We can restate the counting problem by noticing that the total number of defined cycles amounts to $3M + 3M + 3 = 6M + 3 = 3g$. However, the total number of identities is given by $2(M - 1) + 3 = g$ and hence the number of independent cycles is once more $4M + 2 = 2g$ as expected.

The generalized dimer method amounts to writing the partition function as a sum of 2^{2g} G-invariant Pfaffians associated to all possible different orientations Φ.

We call *fundamental* orientation Φ_F that for which $\Phi(\boldsymbol{a}) = 1$ for all $\boldsymbol{a} \in H_1(\Sigma, \boldsymbol{Z_2})$. This can be obtained by setting

$$\phi_i(n_1, n_2, n_3) = (-1)^{n_i}. \tag{33}$$

While the fundamental orientation makes no distinction among plaquettes, the *antifundamental* Φ_A requires $\Phi_i(q) = -1$ for all E, O cycles but $\Phi(R_i) = 1$. There is no simple recipe for Φ_A analogous to (33) since the way it appears depends on the spanning tree $\mathcal{T}$.

6. Topological intersections and sign functionals

6.1. Intersection of cycles

The bilinear symmetric functional $I[\boldsymbol{a}, \boldsymbol{b}]$ over the cycles $\boldsymbol{a}, \boldsymbol{b}$ is given by $\mathrm{Mod}(p, 2)$ where p is the number of intersections of $\boldsymbol{a}, \boldsymbol{b}$ over Σ. In our case a detailed analysis shows that cycles $\in E, O$ of the same parity or the same normal do not intersect. The general formula can be deduced from

$$I[E_1(m_1, m_2, m_3), O_2(n_1, n_2, n_3)] = \delta_{n_1,m_1-1}\delta_{m_2,n_2-1}\delta_{n_3,m_3+1} \tag{34}$$

by imposing invariance under cyclic permutation of the axes and under the S, T_i symmetry operations. Two adjacent cycles do not intersect.

The cycles R_i do not obey this rule and the intersections with the exceptional cycles are given by

$$\begin{aligned}
&I[R_k, E_i(q)] = 0 \qquad \text{if} \quad i \neq k \\
&I[R_k, O_i(q)] = 0 \qquad \text{if} \quad i \neq k \\
&I[R_1, E_i(n_1, n_2, n_3)] = \delta_{i,1}(\delta_{n_2,0}\delta_{n_3,0} + \delta_{n_2,N_2-1}\delta_{n_3,N_3-1}) \\
&I[R_1, E_i(n_1, n_2, n_3)] = \delta_{i,2}(\delta_{n_1,0}\delta_{n_3,0} + \delta_{n_1,N_1-1}\delta_{n_3,N_3-1}) \\
&I[R_1, E_i(n_1, n_2, n_3)] = \delta_{i,3}(\delta_{n_1,0}\delta_{n_2,0} + \delta_{n_1,N_1-1}\delta_{n_2,N_2-1})
\end{aligned} \tag{35}$$

together with the expressions obtained by interchanging E with O.

The definition of $I[\boldsymbol{a}, \boldsymbol{b}]$ can be extended by linearity mod 2 to arbitrary pairs of cycles $\boldsymbol{a}, \boldsymbol{b}$.

6.2. Topological excitation and signature

The intersection formalism leads naturally to the notion of elementary topological excitations $\{\tau_i(q)\}$, a set of minimal operators which locally change a proper orientation into a new one, still proper but inequivalent. τ only acts on the inherited bonds and we can define τ directly over Σ. Any two inequivalent proper orientations are connected by a sequence of τ operations and hence $\{\tau_i(q)\}$ generate all orientations of Σ. In particular, we may reach any orientation by repeatedly applying $\tau_i(q)$ to Φ_0. In the following we use the equivalent notations $\Phi_i(n_1, n_2, n_3) \equiv \Phi_i(q) \equiv \Phi(\boldsymbol{a})$, where $\boldsymbol{a} = E_i(q)$ or $O_i(q)$. The elementary topological excitations are in one-to-one correspondence with the E, O cycles and we may adopt the same set of indices and distinguish between even or odd excitations, $\tau_i(q) \to \tau_i^E(q), \tau_i^O(q)$.

The action of $\tau_1^E(n_1, n_2, n_3) = \tau_1^E(n_1 - 1, n_2, n_3)$ is given by

$$\phi_1(n_1 - 1, n_2 + \epsilon, n_3 + \xi) \to -\phi_1(n_1 - 1, n_2 + \epsilon, n_3 + \xi) \qquad \epsilon, \xi = 0, 1. \tag{36}$$

The definition extends in an obvious way to the other directions and, in virtue of the invariance under the S, T_i operations, (36) also holds for odd operators. Clearly, the values of ϕ on bonds not appearing in (36) are unaffected by $\tau_1^E(q)$.

Given an elementary cycle, e.g. $E_1(q)$, there exist four other intersecting cycles, e.g.

$$\begin{aligned}
&O_2(D_1^{-1}D_2D_3^{-1}q) \qquad O_2(D_1^{-1}D_2D_3q) \\
&O_3(D_1^{-1}D_2^{-1}D_3q) \qquad O_3(D_1^{-1}D_2D_3q).
\end{aligned} \tag{37}$$

Consider now the orientation $\Phi_2(n_1 - 1, n_2 + 1, n_3 - 1)$ corresponding to $O_2(n_1 - 1, n_2 + 1, n_3 - 1) = O_2(D_1^{-1}D_2D_3^{-1}q)$,

$$\begin{aligned}
\Phi_2(n_1 - 1, n_2 + 1, n_3 - 1) &= \phi_1(n_1 - 1, n_2 + 1, n_3 - 1)\phi_3(n_1, n_2 + 1, n_3 - 1) \\
&\times\phi_{-1}(n_1, n_2 + 1, n_3)\phi_{-3}(n_1 - 1, n_2 + 1, n_3).
\end{aligned} \tag{38}$$

The last factor changes sign under the action of $\tau_1^E(q)$ and hence the orientation of $\Phi_2(n_1-1, n_2+1, n_3-1)$ also changes and the same result holds for the other cycles of example (37).

The action of $\tau_i^{E,O}(q)$ changes Φ into an inequivalent orientation which differs from Φ only in the orientations of the local cycles intersecting $E_i(q)$, $O_i(q)$. The orientation of all faces of Σ remain unchanged under $\tau_i^{E,O}(q)$ so that the Kasteleyn conditions are always fulfilled. Each cycle can be given an active role if identified with $\tau_i^{E,O}(q)$ or a passive one if considered as a cycle changing parity under the action of $\tau_i^{E,O}(q)$. The functional $\mathcal{I}_{\boldsymbol{a}} \in H^1(\Sigma, \boldsymbol{Z_2}) : H_1(\Sigma, \boldsymbol{Z_2}) \to \boldsymbol{Z_2}$ is defined by

$$\mathcal{I}_{\boldsymbol{a}}(\boldsymbol{b}) = (-1)^{I[a,b]} \boldsymbol{a}, \boldsymbol{b} \in H_1(\Sigma, \boldsymbol{Z_2}). \tag{39}$$

6.3. Axial gauge

We fix the gauge for the orientations of bond by selecting a subset of $N-1$ bonds forming a spanning tree $\mathcal{T}$ of Λ, that contains all the sites of Λ. A convenient gauge fixing is the axial gauge (as displayed in figure 4):

$$\begin{aligned}
&\phi_3(0,0,n_3) = 1 \qquad n_3 = 0, 1, \ldots, N_3 - 2 \\
&\phi_2(0,n_2,n_3) = (-1)^{n_3} \qquad n_2 = 0, 1, \ldots, N_2 - 2 \qquad n_3 = 0, 1, \ldots, N_3 - 1 \\
&\phi_1(n_1,n_2,n_3) = (-1)^{n_1} \qquad n_1 = 0, 1, \ldots, N_1 - 2 \\
&n_2 = 0, 1, \ldots, N_2 - 1 \qquad n_3 = 0, 1, \ldots, N_3.
\end{aligned} \tag{40}$$

The axial gauge leaves undetermined the orientations of $3N-(N-1) = 2N+1 = 16M+1$ bonds not belonging to $\mathcal{T}$. However, the $12M-1$ Kasteleyn conditions reduce the number of such independent orientations to $16M+1-12M+1 = 4M+2 = 2g$, as expected.

From the recursive relation equivalent to (10)

$$\Phi(\boldsymbol{a}+\boldsymbol{b}) = \Phi(\boldsymbol{a})\Phi(\boldsymbol{b})(-1)^{I[a,b]} \tag{41}$$

we deduce then the value of Φ on all the elements of $H_1(\Sigma, \boldsymbol{Z_2})$ starting from $\Phi_i(q)$. From (10) we see that $\Phi_i(q)$ is invariant under $\mathcal{G}$ and the same is therefore true for all $\Phi(\boldsymbol{a})$. The set of all the $\Phi_i(q)$ determines therefore the global orientation $\Phi \pmod{\mathcal{G}}$ of Σ.

7. General procedure and Pfaffian expansion over Σ

The geometrical structure on which we define Pfaffians admits an alternative equivalent definition. We consider two cubic lattices Λ_E, Λ_O each having M vertices in one-to-one correspondence with even/odd cubes $C(n_1, n_2, n_3)$ where $n_1+n_2+n_3 =$ even/odd, respectively. The bonds of the lattices correspond to the even/odd E, O cycles.

In place of spins we have the orientation parity of the E, O cycles, satisfying the identities (26)–(29). Topology plays a marginal role in the classical 2D Ising lattice where the genus $g = 1$ leads to a sum over four Pfaffians only.

Here the reduction of the original sum on $N = 4(g-1)$ spins to one on $2g$ functionals does not solve the problem but reduces the complexity of the task. The orientations on the sublattices Λ_E, Λ_O are not independent.

We now sketch the general algorithm which fixes all gauges and gives all bond orientations $\phi_i(q)$ in terms of a subset of $2g$ independent ϕ' by means of the Kasteleyn conditions. We consider anly the homogeneous case where the activities of bonds are the same in all directions, however, the results can be straightforwardly generalized to any non-homogeneous distribution of bond interaction energies.

The actual steps are quite complex and can be summarized as follows:

(1) Compile a list of all $3N$ $\phi_i(q)$ considered as independent binary variables.
(2) Impose the axial gauge (40) and obtain a sublist of $2N+1$ terms $\phi_i(q)$ only.
(3) Impose the Kasteleyn conditions over faces. This can be achieved by solving iteratively (8) thus reducing the number of independent $\phi_i(q)$ to $2g = 2 + N/2$ forming a basis $\mathcal{B}$ for the 2^{2g} functionals in $H^1(\Sigma, \boldsymbol{Z_2})$. From $\mathcal{B}$ we define by group multiplication the generic functional $\Phi(\boldsymbol{a}) \in H^1(\Sigma, \boldsymbol{Z_2})$, $\forall \boldsymbol{a} \in H_1(\Sigma, \boldsymbol{Z_2})$.
(4) Select a complete basis $\Omega = \{\omega_k, k = 1, \ldots, 2g\}$ of independent cycles out of E, O, R_1, R_2, R_3. A generic cycle can then be written as

$$\boldsymbol{a} = \sum_{k=1}^{2g} e_k \omega_k \qquad e_k = 0, 1. \tag{42}$$

(5) Define the self-intersection function $H_1(\Sigma, \boldsymbol{Z_2}) \to \boldsymbol{Z}_2$, see (34), (35), (41)

$$\sigma(\boldsymbol{a}) = (-1)^{\sum_{k=2}^{2g} \sum_{k'=1}^{k-1} I[\omega_k, \omega_{k'}] e_k e_{k'}}. \tag{43}$$

(6) The function $\mathcal{I}_{\boldsymbol{a}}$ in (39) defines an invertible duality map $H_1(\Sigma, \boldsymbol{Z_2}) \to H^1(\Sigma, \boldsymbol{Z_2})$. The map $\sigma \circ \mathcal{I}_{\boldsymbol{a}}^{-1}$ lifts the self intersection to $H^1(\Sigma, \boldsymbol{Z_2})$. In any case we do not need to compute explicitly the inverse of $\mathcal{I}_{\boldsymbol{a}}$.
(7) Given $\boldsymbol{a}$ as in (42), we compute $\mathcal{I}_{\boldsymbol{a}}$ and expand it in terms of the restricted basis $\mathcal{B}$ defined in step 3, thus determining the orientations $\Phi(\boldsymbol{a})$, $\phi_i(q)$ and all matrix elements of $M(\Phi(\boldsymbol{a}))$ explicitly as functions of $e_1, \ldots, e_{2g}$.
(8) The dimer generating function $\boldsymbol{Z}_0(X)$ is then given by the sum over Pfaffians

$$\begin{aligned} \boldsymbol{Z}_0(X) &= \frac{1}{2^g} \sum_{\boldsymbol{a} \in H_1} \sigma(\boldsymbol{a}) \boldsymbol{Pf}(\Phi(\boldsymbol{a}), X) \\ &= \frac{1}{2^g} \sum_{\{e_k = 0,1\}} (-1)^{\sum_{k=1}^{2g} \sum_{k'=1}^{k-1} I[\omega_k, \omega_{k'}] e_k e_{k'}} \boldsymbol{Pf}\left(\Phi\left(\sum_{k=1}^{2g} e_k \omega_k\right), X\right). \end{aligned} \tag{44}$$

As in equation (4), the Ising partition function is simply given by

$$Z = (2\cosh(\beta J))^{3N} \boldsymbol{Z}_0(X) \tag{45}$$

where J is the spin–spin interaction energy and $X = \tanh(\beta J)$ is the activity of a bond at inverse temperature β.
(9) For non-bipartite lattices such as the decorated spin lattices there is no direct and fast numerical method to compute Pfaffians with their proper sign. This is possible in other cases, for example in dimer coverings of bipartite lattices where the matrix $M(\Phi(\boldsymbol{a}))$ is block diagonal. In spin lattices we first compute the determinant of M, extract the positive root and set $\boldsymbol{Pf}(\Phi, 0)$ positive. The sign at $X = 1$ is then directly given by $\sigma(\boldsymbol{a})$ or obtained by analytic continuation of the Pfaffian which is a polynomial of degree $3N$ in X. Thus $\sigma(\boldsymbol{a})$ could be used to predict the parity of the number of real zeros of the Pfaffian in the interval $0 < X < 1$.

8. Preliminary analysis of Pfaffians

This section is very preliminary and deals with a number of properties and conjectures which will need to be discussed in detail in a separate study [27]. However, we anticipate some simple results which are essential in analysing the behaviour of the Pfaffian expansion.

Some of these properties have been verified on finite Ising lattices and are in agreement with extensive numerical sampling and numerical findings [21]. We should mention that the

procedure has not yet been optimized for a numerical approach. In particular, the classification of Pfaffian symmetries has still to be implemented.

The self-intersection function $\sigma(\boldsymbol{a})$ can be defined on any triangulated surface of genus g and particular examples of genus $g = 0$ to 3 have been worked out in detail in the literature [4, 13]. The argument $\boldsymbol{a}$ takes 2^{2g} values parametrized by $2g$ binary variables $e_1, \ldots, e_{2g}$. It is always possible to redefine the basis in $H_1(\Sigma, \boldsymbol{Z_2})$ in such a way as to have $\sigma(\boldsymbol{a}) = (-1)^{\sum_{i=1}^{g} e_i e_{i+g}} = \prod_{i=1}^{g} (-1)^{e_i e_{i+g}}$. The factor $(-1)^{e_i e_{i+g}}$ takes a value of 1 three times and a value of -1 once as e_i, e_{i+g} run on 0, 1 and all the factors appearing in $\sigma(\boldsymbol{a})$ are independent. Suppose now that $N_+(g)$, $N_-(g)$ are the number of times $\sigma(\boldsymbol{a})$ takes the values $1, -1$ respectively, so that $N_+(1) = 3$ and $N_-(1) = 1$. We have the recursion relation

$$N_+(g+1) = 3N_+(g) + N_-(g) \qquad N_-(g+1) = N_+(g) + 3N_-(g) \tag{46}$$

which has the solution

$$N_+(g) = 2^{g-1}(2^g + 1) \qquad N_-(g) = 2^{g-1}(2^g - 1). \tag{47}$$

$N_+(g)$ and $N_-(g)$ give the total number of positive and negative $\sigma(\boldsymbol{a})$ in expansion (44). This statistics is important in evaluating the convergence properties of the expansion. For high g this means that if we pair-off positive and negative $\sigma(\boldsymbol{a})$ we are left with a small excess of 2^g positive values, i.e. one part in 2^g. Since $\boldsymbol{Pf}(\Phi, 0) = 1$ we have $\boldsymbol{Z}_0(0) = 1$ as expected at $T = \infty$. As X increases all terms in (44) eventually become positive and equal to $\boldsymbol{Pf}(\Phi_F, 1)$. Comparing the total sum $2^{2g}\boldsymbol{Pf}(\Phi_F, 1)$ with the known $T \to 0$ limit for $\boldsymbol{Z}_0$ we obtain $\boldsymbol{Pf}(\Phi_F, 1) = 2^{14M}$. The equality of the absolute values of $\boldsymbol{Pf}(\Phi, 1)$ only holds on decorated spin lattices whereas generic dimer lattices have a spectrum of values. The factor $\sigma(\boldsymbol{a})$ induces a cancellation with a cutoff factor 2^{-g} in (44) in the $T \to \infty$ or $X \to 0$ limit which does not occur at $T \to 0$ and leads to a steeper log derivative for $\boldsymbol{Z}_0(X)$ as compared with that of the single Pfaffians.

As first noted by Kramers and Wannier [19], planar spin lattices can be characterized by duality relations. However, for $g > 0$ duality does not directly relate the partition function of a lattice to that of the dual, but rather acts very simply on the single terms in expansion (44) by only changing their signs so that they are still positive in the $T \to \infty$ limit. Since duality swaps $T \to \infty$ and $T \to 0$ limits we see that in dual lattices positivity is required at opposite ends of the interval $0 < X < 1$. In the 2D Ising lattice the sign reversal does not alter the partition function in the thermodynamical limit but the same need not to be true in three dimensions. In any case the 3D lattice is not self-dual.

A lower bound X_0 for the zeros of $\boldsymbol{Pf}(\Phi, X)$ can be derived from (16). From the spectrum of A_f, B_f we get $\|A_f\| < 2+\sqrt{3}$, $\|B_f\| < 2+\sqrt{3}$, whence $X_0 > \frac{1}{2+\sqrt{3}} = 2-\sqrt{3} \simeq 0.267\ldots$. Numerical analysis indicates that in fact Pfaffians vanish in the range $X_m = 0.3178\ldots$ which is actually reached by $\boldsymbol{Pf}(\Phi_F, X)$ to $X_M = 0.3506\ldots$ reached by $\boldsymbol{Pf}(\Phi_A, X)$. These values can be computed exactly as roots of an algebraic equation because the translational symmetry of these Pfaffians leads to explicit formulae. Random sampling of orientations Φ up to $N_1 = N_2 = N_3 = 8$ indicate that zeros tend to accumulate around 0.34, see figure 5.

Therefore, we now divide the interval $0 < X < 1$ into 4 regions:

(i) The very low temperature region $X > X_M$ where all terms in expansion (44) of $\boldsymbol{Z}_0$ are positive and the series converges rapidly and agrees with low-T expansions.

(ii) The crossover region centred at $X = 0.34$, where $N_-(g) = 2^{g-1}(2^g - 1)$ Pfaffians change sign.

(iii) The region between the estimated critical temperature $X = X_0 \simeq 0.218\,0945(2)$ [22] and X_m. In this region the negative terms have absolute values smaller that the positive terms and we expect that convergence degrades rapidly as we move toward X_0.

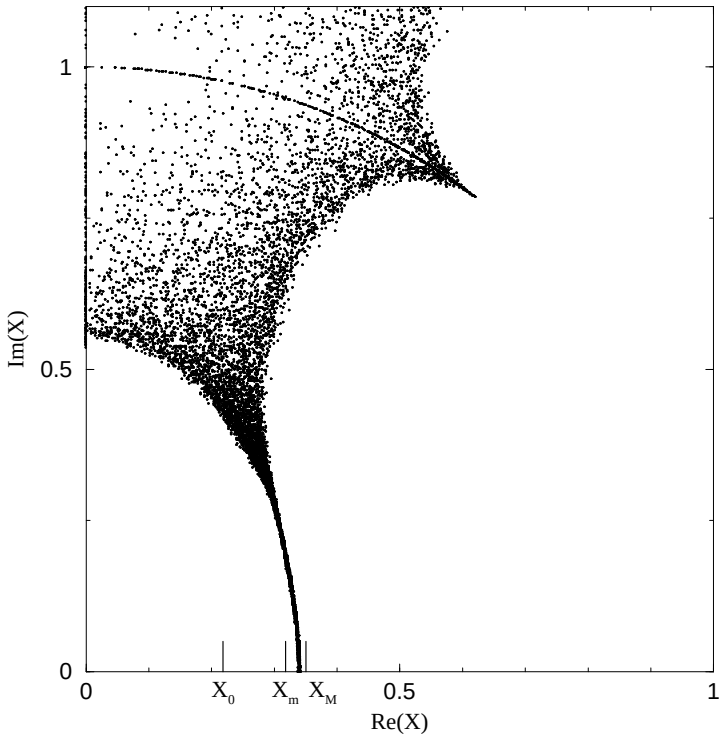

Figure 5. Overlap of the complex zeros of 50 Pfaffians corresponding to different randomly chosen orientations ($N_1 = N_2 = N_3 = 8$). X_M and X_m (computed in the $N \to \infty$ limit) are the upper ond lower bounds for the zeros given by the singularities of the fundamental and antifundamental Pfaffians, respectively. X_0 corresponds to the value of the critical temperature estimated by different analytical and numerical methods.

(iv) The high-temperature region $X < X_0$ where all absolute values of the terms in (44) become comparable and the value of $\boldsymbol{Z}_0$ is determined by 2^g unpaired Pfaffians. For small X all absolute values of the Pfaffians are close to 1 and the sum (44) over a sample of L random terms has a noise of the order of $2^{-g}\sqrt{L}$ while we expect a signal of the order of $2^{-2g}L$, normalized to 1 at $X = 0$ for the complete sum. In order to get a signal we need a signal/noise ratio $\frac{2^{-2g}L}{2^{-g}\sqrt{L}} \simeq 1$, i.e. $L \simeq 2^{2g}$. This means that unless one sums over all terms we only get noise and that numerical computation is ruled out unless one obtains an explicitly summable formula for the Pfaffians as happens in the limit $T \to \infty$. Therefore, exact matching with known $T \to \infty$ results is still possible and useful. As X increases the absolute values of the positive terms grows, on average, more rapidly than that of the negative ones thus improving the signal/noise ratio. We conjecture that the critical $X = X_0$ is effectively a threshold beyond which the signal becomes effective. In general, for a fixed X and all Φ we have $\boldsymbol{Pf}(\Phi_A, X) \leqslant \boldsymbol{Pf}(\Phi, X) \leqslant \boldsymbol{Pf}(\Phi_F, X)$.

Further details and high/low temperature expansion will be discussed in a forthcoming paper [27].

9. Dimer statistics

A simple application of the above formalism is the evaluation of the number of perfect matchings, i.e. dimer coverings, over the 3D cubic lattice Λ.

As for the Ising model, it can be solved exactly or treated easily in the case of planar lattices, whereas it still represents an open problem in the case of non-planar graphs [23].

The dimer-covering generating function is given by a Pfaffian expansion similar to (44) where $M(\Phi)$ is now a $N \times N$ matrix of elements $M_{q,q'}(\Phi) = \phi_i(q) = \pm 1$ depending on the orientation of the bond. The decorating bonds are absent whereas the orientations Φ of Σ play exactly the same role as in the Ising case. Following the same steps discussed for the Ising case and separating odd and even sites, we arrive to a block diagonal form of $M(\Phi)$:

$$M(\Phi) = \begin{pmatrix} 0 & C(\Phi) \\ -C(\Phi)^T & 0 \end{pmatrix}. \tag{48}$$

We now have directly $\boldsymbol{Pf}(M(\Phi)) = \mathrm{Det}(C(\Phi))$, and the expansion reads

$$\begin{aligned} \boldsymbol{Z}_{\mathrm{Dimers}} &= \frac{1}{2^g} \sum_{\boldsymbol{a} \in H_1} \sigma(\boldsymbol{a}) \boldsymbol{Pf}(\Phi(\boldsymbol{a})) = \frac{1}{2^g} \sum_{\{e_k = 0,1\}} (-1)^{\sum_{k=2}^{2g} \sum_{k'=1}^{k-1} I[\omega_k, \omega_{k'}] e_k e_{k'}} \mathrm{Det}(C(\Phi)) \\ \Phi &\equiv \Phi\left(\sum_{k=1}^{2g} e_k \omega_k \right). \end{aligned} \tag{49}$$

Such a formula can be used both for exhaustive enumerations of coverings $h(N_1, N_2, N_3)$ of finite lattices of linear size $N_1 \times N_2 \times N_3$ as well as in a probabilistic framework [27].

We have applied (49) to the case of finite cubic lattices with open boundaries in order to recover and improve the known results. The limitations in the size arise from the number of terms appearing in the expansion which increase exponentially with the genus of the surface, which for open boundaries grows as $g = M_1M_2(M_3 - 1) + M_2M_3(M_1 - 1) + M_3M_1(M_2 - 1) - M_1M_2M_3 + 1$ ($g = 2L^3 - 3L^2 + 1$ in the isotropic case of linear size L). We have found $h(4, 4, 4) = 5051\,532\,105$ (in agreement with [25]), $h(6, 4, 4) = 932\,814\,464\,901\,633$ and $h(6, 6, 4) = 123\,115\,692\,449\,982\,216\,049\,513$.

Note that the rigorous lower bound [24] on the number of dimer coverings in three dimensions in the $M \to \infty$ limit can be easily recovered in our approach by computing, via Fourier transform, the periodic Pfaffian corresponding to Φ_F [27].

Equation (49) can be also thought of as the expansion in terms of determinants of the permanent of 0–1 matrices, a $\#P$-complete problem which can be easily mapped onto the evaluation of dimer coverings over an associated bipartite lattice [26].

10. Conclusion

In this paper we propose a combinatorial/topological formalism for the study of the Ising problem over lattices of arbitrarily high topological genus which generalizes the well known approach of Kasteleyn. The partition function is written as a sum over Pfaffians with a topological signature.

We apply the method to the 3D cubic Ising problem where we have reached a very preliminary assessment on the expansion in the high- and low-temperature ranges. The same formalism applies to the perfect matchings problem and provides a determinant expansion for the permanent of 0–1 matrices.

Work is in progress on the physical and algorithmic relevance of the method.

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