On the Dimer Problem and the Ising Problem in Finite 3-dimensional Lattices.

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January 2, 2001

Abstract

We present a new expression for the partition function of the dimer arrangements and the Ising partition function of the 3-dimensional cubic lattice. We use the Pfaffian method. The partition functions are expressed by means of expectations of determinants of matrices naturally associated with the cubic lattice.

The dimer problem and the Ising problem. The *close-packed dimer model* of statistical mechanics can be stated as follows. One considers a set of sites and a set of bonds connecting certain pairs of sites. Each bond b can absorb a 'dimer' (which represents a diatomic molecule) with corresponding energy E_b. It is required that each site is occupied exactly once by one of the atoms of a dimer. A state s is an arrangement of dimers which meets this requirement, and its energy $E(s)$ is $\sum E_b$ where the sum is taken over

*Partially supported by the Project LN00A056 of the Czech Ministery of Education, by GAUK 158 grant, and by FONDAP on applied mathematics; currently visiting School of Mathematics, Georgia Institute of Technology, Atlanta, GA 30332-0160, U.S.A.

all bonds b which absorb a dimer. Then the partition function of the dimer model may be viewed as a density function of energy levels.

The dimer model was first considered by Roberts [1] in 1935, and by Fowler and Rushbrook [2]. The dimer model for 2-dimensional lattices appears in calculations of the thermodynamic properties of a system of diatomic molecules-dimers. It has been solved by Kasteleyn [3] and by Temperley and Fisher [4]. The same problem for 3-dimensional lattices remains an important open problem of statistical physics (see [5] for references).

Many fundamental observations about the dimer and monomer-dimer model in general lattice graphs have been given by Heilmann and Lieb [6], [7].

Another model we consider here is the *Ising version of the Edwards-Anderson model*. It can be described as follows. A *coupling constant* J_{ij} is assigned to each bond $\{i, j\}$ of a given lattice graph G; the coupling constant characterizes the interaction between the particles represented by sites i and j. A physical state of the system is an assignment of spin $\sigma_i \in \{+1, -1\}$ to each site i. The *Hamiltonian* (or energy function) is defined as $H(\sigma) = -\sum_{\{i,j\}\in E} J_{ij}\sigma_i\sigma_j$. The distribution of physical states over all possible energy levels is encapsulated in the *partition function* $Z(\beta) = \sum_\sigma e^{-\beta H(\sigma)}$ from which all fundamental physical quantities may be derived.

The literature on the 3-dimensional dimer problem and the 3-dimensional Ising problem is vast but there is general feeling and some evidence (see e.g. [8]) that no closed solution similar to the solutions of the 2-dimensional case nor a deterministic efficient algorithm may be found for the cubic lattices.

This however does not rule out a statistical treatment. We believe that our new expressions are natural enough to allow such further analysis.

Recent papers [9], [10] also study the problems using a Pfaffian method. They obtain new expressions by means of a series of Pfaffians with a topological signature. Our approach is more combinatorial in nature. We express the partition functions by means of expectations of the determinants of matrices naturally associated with the cubic lattice. Determinants and spectral properties of random matrices are extensively studied (see e.g. [11]) and a goal of this letter is to draw attention to possible applications of related machinery to the 3-dimensional statistical mechanics problems.

We may reformulate the dimer problem and the Ising problem in graph theoretic terms as follows. A graph is a pair $G = (V, E)$ where V is a set of *vertices* and E is a set of unordered pairs of elements of V, called *edges*.

A graph with some regularity properties may be called a *lattice graph*. We associate with each edge e of G a weight $w(e)$ and for a subset of edges $A \subset E$, $w(A)$ will denote the sum of the weights $w(e)$ associated with the edges in A.

A subset of edges $P \subset E$ is called *perfect matching* or *dimer arrangement* if each vertex belongs to exactly one element of P. The dimer partition function may be viewed as polynomial $\mathcal{P}(G, x)$ which equals the sum of $x^{w(P)}$ over all perfect matchings P of G.

The Ising partition function is very close to the *generating function of cuts* which is a standard concept in graph theory. A *cut* of a graph $G = (V, E)$ is a partition of its vertices into two disjoint subsets $V_1, V_2 \subset V$, and the implied set of edges between the two parts:

$$C(V_1, V_2) = \{\{u, v\} \in E : u \in V_1, v \in V_2\}$$

The *generating function of cuts* $\mathcal{C}(G, x)$ equals the sum of $x^{w(C)}$ over all cuts C of G.

If we set the coupling constant J_{ij} as the weight $w(\{i, j\})$ of the edge $\{i, j\}$, the generating function of cuts becomes very similar to the partition function:

$$Z(\beta) = 2 \sum_{cut C} e^{-\beta(2w(C)-W)} = 2e^{\beta W} \mathcal{C}(G, e^{-2\beta})$$

where W is the sum of all the edge weights.

3-dimensional cubic lattices. This letter studies properties of finite cubic lattices. Let us now fix notation for them. Let m be odd positive integer and k even positive integer. The cubic lattice $Q_{m,m,k}$ is the following graph:

Q_{mmk} has vertices V_{xyz}, $x, y = 1, ..., m$, $z = 1, ..., k$, and the following edges:

1. The *vertical* edges $v_{xyz} = \{V_{xyz}, V_{xy(z+1)}\}$,
   $z = 1, ..., k-1$,
2. The *width* edges $w_{xyz} = \{V_{xyz}, V_{x(y+1)z}\}$,
   $y = 1, ..., m-1$,
3. The *horizontal* edges $h_{xyz} = \{V_{xyz}, V_{(x+1)yz}\}$,
   $x = 1, ...m-1$.

Let us denote the ordered set $(V_{xy1}, ..., V_{xyk})$ by V_{xy}. V_{xy} will also stand for the vertical path of Q_{mmk} from V_{xy1} to V_{xyk}.

Q_{mmk} is a bipartite graph, which means that its vertices may be partitioned into two sets Z_1, Z_2 such that if e is an edge of Q_{mmk} then $|e \cap Z_1| = |e \cap Z_2| = 1$. Moreover, we have also that $|Z_1| = |Z_2| = mmk/2$. Let $\mathcal{Z}$ be square $(Z_1 \times Z_2)$ matrix defined by $\mathcal{Z}_{ij} = x^{w(ij)}$ if ij is an edge of Q_{mmk} and $\mathcal{Z}_{ij} = 0$ otherwise.

We will consider matrix $\mathcal{Z}$ with its rows and columns ordered in aggreement with the *natural order* $(V_{11}, V_{12}, ..., V_{1m}, V_{21}, ..., V_{mm})$ and we will assume that $V_{111} \in Z_1$.

Note that $\mathcal{P}(Q_{mmk}, x)$ equals the permanent of $\mathcal{Z}$. In this letter we show that $\mathcal{P}(Q_{mmk}, x)$ may be computed from the average of determinants of CERTAIN signings of $\mathcal{Z}$, where a *signing* of a matrix is obtained by multiplying some of the entries of the matrix by -1.

The signings of $\mathcal{Z}$ correspond to orientations of Q_{mmk}.

An *orientation* of a graph $G = (V, E)$ is a *digraph* $D = (V, A)$ obtained from G by assigning an orientation to each edge of G, i.e., by ordering the elements of each edge of G. The elements of A are called *arcs*. We say that signing Z of $\mathcal{Z}$ corresponds to orientation D of Q_{mmk} if $Z_{ij} = x^{w(ij)}$ if $(ji) \in A(D)$, $Z_{ij} = -x^{w(ij)}$ if $(ij) \in A(D)$, and $Z_{ij} = 0$ otherwise.

An expression of similar flavour as our result exists already: a seminal observation of Heilmann and Lieb [6], [7] asserts that $\mathcal{P}(Q_{mmk}, x)$ equals the average of $(det(Z))^2$ over ALL signings Z of $\mathcal{Z}$.

A difference of our expression with the result of Heilmann and Lieb is that we replace the average of a multiquadratic function by the average of a multilinear function, with a restricted range.

Statement of the main result. An orientation D of Q_{mmk} is called *stable* if all vertical edges are oriented in D in agreement with the natural order. For edge e we let $s_D(e) = 0$ if the orientation of e agrees with the natural order, and $s_D(e) = 1$ otherwise.

Let D be a stable orientation. Then we let $sgn(D) = 1$ if

$$\sum_A s_D(w_{x(2y)z}) s_D(w_{x(2y'-1)z'}) =$$

$$\sum_B s_D(h_{(2x)yz}) s_D(h_{(2x'-1)y'z'})$$

modulo 2 and $sgn(D) = -1$ otherwise, where

$$A = \{(xyzy'z'); 1 \leq x \leq m, 1 \leq y \leq (m-1)/2, 1 \leq z \leq k,$$
$$1 \leq y' \leq y, z \leq z' \leq z+1\}$$

and

$$B = \{(x, y, z, x', y', z'); 1 \leq x \leq (m-1)/2, 1 \leq z \leq k,$$
$$1 \leq y \leq m, 1 \leq x' \leq x,$$
$$(y, z) \leq (y', z') \leq (y'', z'')\}.$$

In the definition of B the order of pairs of integers is lexicographic and (y'', z'') is the immediate successor of (y, z). Let M be unique perfect matching of Q_{mmk} consisting of vertical edges only.

Theorem 1

$$\mathcal{P}(Q_{mmk}, x) = -2^{C_r} x^{w(M)} + \alpha(2^{C_r} + 1)$$

where α equals the average of $det(Z(D))$, D stable orientation of Q_{mmk} with $sgn(D) = +1$, and $C_r = km(m-1)$.

Having the expression for the partition function of the dimer problem given in Theorem 1, let me now briefly indicate how to transform the 3-dimensional Ising problem to the dimer problem of locally modified cubic lattice. This transformation goes back to Kasteleyn [3] and Fisher [12] and it is well described e.g. in [13]. An *eulerian subgraph* of a graph $G = (V, E)$ is a set of edges $U \subset E$ such that each vertex of V is incident with an even number of edges from U. The *generating function of eulerian subgraphs* $\mathcal{E}(G, x)$ equals the sum of $x(U)$ over all eulerian subgraphs U of G. The partition function of the Ising problem of a graph (with zero magnetic field) can be expressed as the generating function of eulerian subgraphs of the same graph, with modified edge variables.This classic relation between the Ising partition function and the generating function of eulerian subgraphs was discovered by van der Waerden [14]:

$$Z(\beta) = 2^n \prod_{\{i,j\} \in E} \cosh(\beta J_{ij}) \quad \mathcal{E}(G, \tanh(\beta J_{ij})).$$

The generating function of eulerian subgraphs of the cubic lattice may be transformed into the generating function of perfect matchings of a locally modified graph Q^*_{mmk}. A Fisher's construction [12] is useful since it is local in the sense that it only modifies each vertex in a way dependent on its degree and it preserves the embedding of Q_{mmk}.

Hence an expression analogous to the one described in this paper for the dimer problem holds for the Ising problem as well. In fact, one should find an analogous expression for the 3-dimensional variants of the problems which may be treated by the Pfaffian method in 2 dimensions, like a variant of the ice problem.

A Theory of Pfaffian Orientations. The proof of our result is involved: this paper may be viewed as a continuation of three papers [15], [16], [13]. A theorem of Galluccio and Loebl [15] expresses $\mathcal{P}(G,x)$, where G is an arbitrary graph, as a linear combination of Pfaffians of matrices associated with *relevant* orientations of G. When G is a bipartite graph like the cubic lattice, the Pfaffians may be turned into determinants. The relevant orientations may be naturally described when the graph is embedded in a certain way on an orientable surface.

This 'Pfaffian approach' to the dimer problem was started by Kasteleyn [3]. Kasteleyn [3] and Fisher [12] also described methods how to find the Ising partition function for a graph G as the dimer partition function of a locally modified G. One such transformation was briefly indicated above. In [16] and [13], the Pfaffian method leads to an efficient algorithmic treatment of the Ising problem for finite lattices which may be embedded on a fixed surface, e.g. on a torus.

We use the Pfaffian method to prove Theorem 1 as follows: we embed the three-dimensional cubic lattice to a 2-dimensional orientable surface, use the theory developed in [15] and finally characterize the coefficients of the resulting linear combination and turn it into a probabilistic expression.

Even though geometry of the cubic lattice plays a key role in the proof, we find it curious that the final result in Theorem 1 is formulated without mentioning it.

A Curious Corollary. Applying elementary probabilistic analysis to the statement of Theorem 1 I have obtained a curious corollary which may be of independent interest. Once discovered, the corollary may be proved directly without using Theorem 1.

Let Q' be a cubic lattice with added boundary edges, i.e. degree of each vertex of Q' is equal to six. A subset C of vertices of Q' is called *cover* if each edge of Q' is incident with exactly one vertex of C. Note that Q' has exactly 2 covers. A subgraph of Q' is called *part* if it is obtained from Q' by deleting both horizontal and/or vertical edges incident with each vertex of a fixed cover C of Q'. Hence each vertex of C has degree 2 or 4 in any part. A part P is called *even* if the number of vertices of C of degree 2 in P is even, and P is called *odd* otherwise.

Theorem 2.

$$\mathcal{P}(Q', x) = \sum_{W \in A} \mathcal{P}(W, x) - \sum_{W \in B} \mathcal{P}(W, x)$$

where A consists of the even parts and B consists of the odd parts.

Proof. Let M be a perfect matching of Q'. We will compute how does M contribute to the RHS. Let Z be the subset of vertices of Q' incident to a vertical edge of M, and let $z = |Z|$. M contributes to a term of the RHS corresponding to a part P if and only if M is a perfect matching of P. Hence, the contribution of M equals $\sum_{i=0}^{z} (-1)^i 2^{z-i} \binom{z}{i}$, which equals $(2-1)^z = 1$ by binomial theorem.

Conclusion. We have expressed the partition functions of the dimer problem and the Ising problem in 3-dimensional finite cubic lattices by means of expectations of the determinants of matrices naturally associated with the cubic lattices. This may open a possibility to apply fundamentally different statistical methods and Monte Carlo simulations to study these problems.

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