A Pfaffian formula for monomer-dimer partition functions

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The monomer-dimer covering problem shows up in several areas of physics and other fields. While the partition function of the pure dimer covering problem on planar lattices was solved ages ago by Kasteleyn and Fisher-Temperley in terms of Paffians (whose squares are easily computable determinants), the inclusion of monomers (i.e., vertices uncovered by dimers) is an intractable problem. Together with *Alessandro Giuliani and Ian Jauslin* we have succeeded in utilizing an ancient theorem* to write the partition function of a restricted monomer-dimer problem as a Pfaffian. This is the model in which *monomers are allowed on the boundary vertices of an arbitrary planar graph.*

*J. Combinatorial Theory 5, 313-319 (1968).

Monomer Dimer Covering

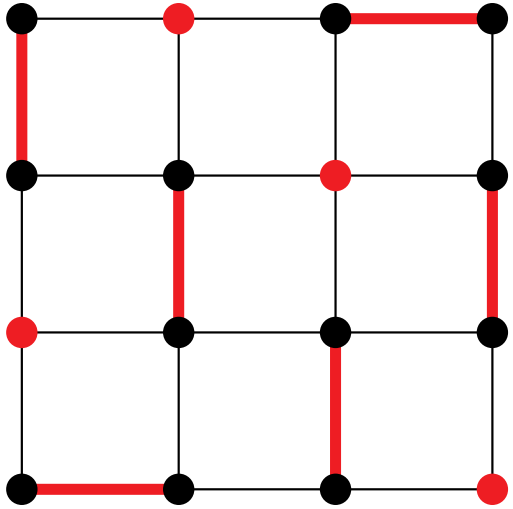
We are given a graph, which means a collection of points (called vertices) and a collection of bonds (or edges) connecting pairs of vertices. Each bond may carry a 'weight' W_{ij}, which often is just 1. A graph is planar if it can be drawn in a plane without any crossing of edges.

A (pure) dimer covering is a choice of the edges and their end-point vertices so that every vertex is covered exactly once. This is also called a 'matching'. The weight associated to a covering is simply the product of the W_{ij}'s on the covered edges.

A monomer-dimer covering is one in which some vertices (called monomers) are left uncovered. We can attach a weight ℓ_j to each vertex, and the weight of an MD covering is then the product of the W_{ij}'s of the covered edges times the product of the monomer weights ℓ_j of the uncovered vertices (i.e., the monomers).

The partition function, Ξ, is then the sum, over all MD coverings, of the weights of the coverings. The usual case is all $W_{ij} = 1$ and all $\ell_j = z = \text{monomer fugacity}$. Our aim is to compute Ξ for planar graphs.

An Example



The faint lines are the edges, the red lines are the dimers (and their endpoints are the black vertices). The red dots are the monomers (or uncovered vertices).

Pfaffians

Given a size-n triangular array of numbers with n even:

$$A = \begin{bmatrix} A_{12} & A_{13} & A_{14} & \cdots & A_{1n} \\ & A_{23} & A_{24} & \cdots & A_{2n} \\ & & A_{34} & \cdots & A_{3n} \\ & & & & \vdots \\ & & & & A_{n-1,n} \end{bmatrix}$$

the Pfaffian of A is defined using a rule similar to that of determinants. For example, when $n = 4$,

$$\mathrm{pf}(A) = A_{12}A_{34} - A_{13}A_{24} + A_{23}A_{14}. \qquad (*)$$

What makes the Pfaffian useful is its relation to a determinant, which is relatively easy to compute. The relation is that

$$\mathrm{pf}(A)^2 = \det(\mathcal{A})$$

where $\mathcal{A}$ is the $n \times n$ antisymmetric matrix formed from A, and its mirror image, and with zeros on the diagonal.

Kasteleyn's theorem

Recall, for $n = 4$,

$$\mathrm{pf}(A) = A_{12}A_{34} - A_{13}A_{24} + A_{23}A_{14}. \qquad (*)$$

We note that the choice $A_{ij} = W_{ij}$ for a graph of 4 vertices gives us the Ξ for $z = 0$, except for the fact that there is an unwanted minus sign in $(*)$. This defect is easily remedied by letting $A_{13} = -W_{13}$, in which case $\mathrm{pf}(A) = \Xi$.

The big question is whether this simple trick can turn a partition function into a Pfaffian for bigger graphs. Obviously, when we put minus signs in one place, we might mess up other places. Kasteleyn's theorem is that this can always be done for planar graphs.

The second big problem is accomodating monomers in the Pfaffian setup. For this purpose, we recall an ancient *Theorem on Pfaffians* (E. Lieb, J. Combinatorial Theory 5, 313-319 (1968)).

Theorem on Pfaffians

Recall the well-known theorem on determinants: $\det(A + \lambda I)$ is a polynomial in λ whose coefficients are the elementary symmetric functions of the eigenvalues, but, more interestingly, the coefficient of λ^{n-k} is the sum of the principle determinental minors of order k. In other words, the coefficient of λ^k is the sum of all the determinants we can get by leaving out $n-k$ rows and the same $n-k$ columns.

What is the analog for Pfaffians? How can we count all the sub-Pfaffians obtained by deleting $n-k$ rows and the same $n-k$ columns from A? If we can do this, it looks like we can compute the MD partition function, because the sum of the sub-Pfaffians of order k correspond to the pure dimer partition function on the complement of k vertices (i.e. k monomers).

The ancient solution of the problem is

$$\boxed{\mathrm{pf}\left(A_{ij} - (-1)^{i+j}\lambda\right) = \sum_k P_{2k}\lambda^k}$$

where P_{2k} is the sum of the Pfaffians of all the $n-2k$ principal triangular sub-arrays of A. Note that, unlike for the determinant, λ appears all over the array and not just diagonally.

The $n = 4$ example

$$\begin{aligned}
\mathrm{pf}(A_{ij} - (-1)^{i+j}\lambda) = \quad & (A_{12}+\lambda)(A_{34}+\lambda) - (A_{13}-\lambda)(A_{24}-\lambda) \\
& +(A_{14}+\lambda)(A_{23}+\lambda) \\
= \quad & A_{12}A_{34} - A_{13}A_{24} + A_{14}A_{23} \\
& +\lambda(A_{12}+A_{13}+A_{14}+A_{23}+A_{24}+A_{34}) \\
& +\lambda^2,
\end{aligned}$$

which is the right answer!

Life is not so simple

While it is true that, by adding $(-1)^{i+j}z^2$, we can compute the generating function for all the sub-Pfaffians, it is a heresy to suppose, however, that the sub-Pfaffians are the dimer partition function of the graph with the monomers removed. It is not at all obvious, and indeed it is not true, that the sub-Pfaffian of a correctly-signed Pfaffian (in the sense of Kasteleyn) is a correctly-signed Pfaffian that will give the right partition function. Only in rare cases will it be so.

It is not difficult to show that we never end up with something bigger than the correct answer, and, therefore, if we use this $(-1)^{i+j}z$ rule, we will get a lower bound to the MD partition function. This fact might be useful in some contexts.

Success!

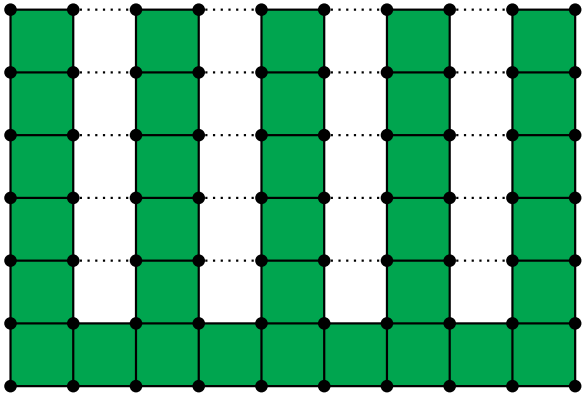
It turns out, that, in certain cases, there are many choices of the Kasteleyn $+$ or $-$ signs that give the correct counting for the pure dimer problem. Among these, there is one, delicately chosen, that yields the correct signage for all the sub-Pfaffians. We can state our result as follows.

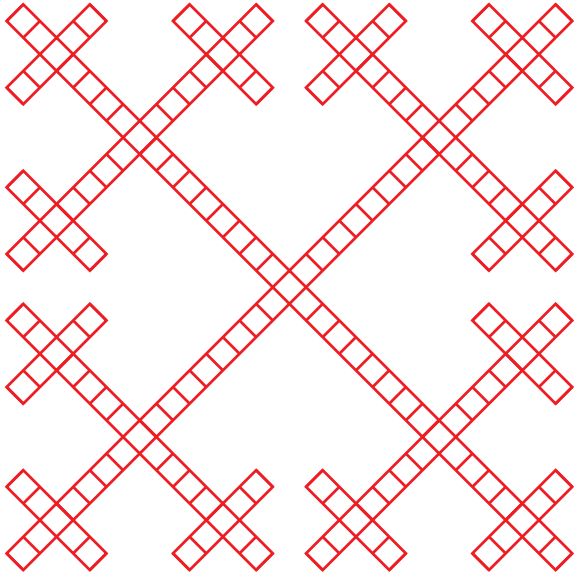
Theorem: Let g be a planar graph, and let ∂g be its boundary, set $\ell_j = 0$ for $j \notin \partial g$, then it is possible to chose the Kasteleyn $\pm$ signs so that

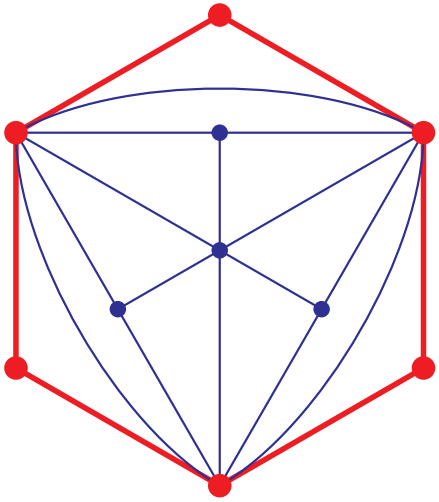
$$\boxed{\mathrm{pf}(A - (-1)^{i+j}\ell_i\ell_j) = \Xi.}$$

In other words, if monomers are allowed on the boundary, then the partition function Ξ is a Pfaffian, and can thus be computed as the square root of a determinant.

Examples







THANKS FOR LISTENING!