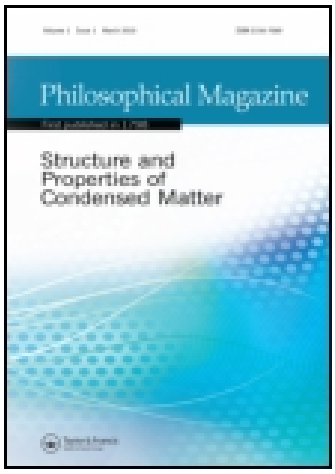

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Dimer problem in statistical mechanics-an exact result

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Dimer Problem in Statistical Mechanics — An Exact Result

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An important, even though physically oversimplified model of a system (e.g. solution or gas) containing diatomic molecules is that of a lattice occupied by 'rigid dimers' (e.g. Fowler and Rushbrooke 1937). Each dimer fills two nearest-neighbour sites on the lattice and no site may be occupied by more than one dimer. This represents a statistical problem of some difficulty which has so far been solved exactly only in one dimension (Green and Leipnik 1960, Fisher and Temperley 1960). (It has been treated by various authors on the basis of approximate statistical methods, e.g. Rushbrooke *et al.* (1953).) This note reports an exact solution for the dimer problem on the plane square lattice in the limiting case where the dimers completely fill the lattice (close-packed or high density limit).

Consider the distribution of dimers on a plane square lattice of m rows and n columns. If $g_{mn}(l, k)$ is the number of ways of placing l horizontal or X-dimers and k vertical or Y-dimers on the lattice then the required configurational grand partition function is

$$Z_{mn}(x, y) = \sum g_{mn}(l, k) x^l y^k \quad . \quad . \quad . \quad . \quad (1)$$

where x and y are the activities of X-dimers and Y-dimers respectively. The numbers of dimers l and k are subject to $l + k = \frac{1}{2}mn$.

For a large lattice

$$Z_{mn}(x, y) \sim [Z(x, y)]^{mn} \quad . \quad . \quad . \quad . \quad . \quad (2)$$

and the free energy per lattice site approaches a limit

$$-(F/kT) = \lim\, (mn)^{-1} \ln Z_{mn}(x, y) = \ln Z(x, y). \quad . \quad . \quad . \quad (3)$$

This is found to be

$$\ln Z(x, y) = \tfrac{1}{2} \ln 2 + (2\pi)^{-2} \int_0^{\pi} \int_0^{\pi} \ln (x^2 + y^2 - x^2 \cos \alpha - y^2 \cos \beta)\, d\alpha\, d\beta. \quad . \quad . \quad . \quad (4)$$

The integral in this result is closely related to Onsager's (1944) expression for the partition function of the asymmetric Ising model *at* the critical temperature T_c. From (4) the free energy and entropy are seen to be continuous smooth functions of the activities x and y and hence of the relative density of X-dimers and Y-dimers. In the symmetric case

$x=y=1$ the integral simplifies and the number of arrangements of N dimers is asymptotically,

$$[Z(1,1)]^{2N}=[\exp(2G/\pi)]^N=(1{\cdot}791623)^N \quad \ldots \quad (5)$$

where $G=1-3^{-2}+5^{-2}-7^{-2}+\ldots=0{\cdot}915\,966$ is Catalan's constant. (The Bethe approximation (Chang 1939) yields the estimate

$$[Z(1,1)]^2\simeq 27/16=1{\cdot}6875.$$

Fowler and Rushbrooke's estimate (1937) was 1·80 which is very close to the exact result.)

The calculation leading to (4) is based on an algebraic property of the Pfaffian. This is a triangular array of numbers filling the spaces above the main diagonal in a determinant. It is evaluated, like a determinant, in terms of the elements of its top row and their corresponding minors, with the same sign conventions. The minor of a_{pq} is now defined by striking out from the Pfaffian both the pth and qth rows *and* columns. This means that each term in the expansion of a Pfaffian of order $2N$ will contain just N factors, and each index p will appear once and once only in such a product. Thus, if we number our $2N$ lattice points in any manner, and put $a_{pq}=x$ when points p and q are horizontal neighbours and $a_{pq}=y$ when p and q are vertical neighbours, all other a's being put equal to zero, it is evident that there will be a 1–1 correspondence between the terms of the Pfaffian and the permissible arrangements of dimers on the lattice of $2N$ points.

As usual in these problems we have to ensure that all the terms are positive. In particular, for the plane square lattice we can take the x's all positive and the y's of alternating signs *or* we can number alternate rows of the lattice in opposite senses. (So far, we have not solved the very much more interesting problem of a lattice with some points empty —the formal 1–1 correspondence can be maintained, but the signs of some of the terms go wrong.)

The Pfaffian has various properties that make it important in mathematical physics. It is, for example, a compact expression for the trace of a product of anticommuting ' Dirac operators ' and its square is the antisymmetric determinant obtained by reflecting the Pfaffian in the main diagonal (Hurst and Green 1960, Caianiello and Fubini 1952). In the present problem, this determinant is almost cyclic and thus can be evaluated, even for a finite lattice with edges, by standard methods, the results closely resembling Kaufman's expressions (1949) for the finite Ising model. By way of example the number of ways of covering an 8×8 chessboard with dominoes has been found to be

$$12\,988\,816=16(901)^2.$$

In the symmetric case $x=y$, the asymptotic expansion is

$$\ln Z_{mn}(1,1)=mn(G/\pi)-(m+n)[\tfrac{1}{2}\ln(1+2^{1/2})-G/\pi]+C+O(m^{-1},n^{-1}) \quad \ldots \quad (6)$$

where C is a constant. The first term in the expression represents the ' bulk ' free energy, whilst the second term is the ' boundary ' free energy and would have a different value if the lattice had been wrapped on a torus. (This possibility can also be dealt with.)

The principal results of this note were discovered independently by the two authors. The detailed derivations are being prepared for publication.

Since completing this work we have heard (private communication) that P. W. Kasteleijn has obtained similar results.

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