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Solution of the dimer problem on a hexagonal lattice with boundary

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Abstract. The dimer problem is solved exactly for a hexagonal lattice with general boundary using a known generating function from the theory of partitions. It is shown that the leading term in the entropy depends on the shape of the boundary.

1. Introduction

Implicit in the notion of a thermodynamic limit is the idea that bulk properties are insensitive to the precise nature of the boundary conditions imposed. An instructive example is provided by the dimer problem on a square lattice. When the dimers are required to occupy every site of the lattice the problem can be solved exactly both for the case of an $m \times n$ rectangular boundary (Fisher 1961, Kasteleyn 1961) as well as for the $m \times n$ torus (Kasteleyn 1961). With either choice of boundary conditions one finds a bulk entropy per dimer:

$$\frac{1}{\frac{1}{2}mn} \log Z \sim \frac{2}{\pi}\left(1-\frac{1}{3^2}+\frac{1}{5^2}-\frac{1}{7^2}+\cdots\right) \qquad m, n \to \infty.$$

In this paper it will be shown that the above statement does *not* hold for the dimer problem on the hexagonal lattice. An exact solution has been known for some time (Wannier 1950, Kasteleyn 1963, Wu 1968 and Nagle 1975) but only for the case of toroidal boundary conditions where one does obtain a bulk entropy (N = number of dimers):

$$\frac{1}{N} \log Z \sim \frac{2}{\pi}\int_0^{\pi/3} \log(2\cos x)\, dx \qquad N \to \infty$$
$$= 0.338\,314. \tag{1}$$

If instead the problem is formulated in a general hexagonal region (to be described below) it is seen to be equivalent to the combinatorial problem of 'plane partitions' (MacMahon 1916 and Chaundy 1931). Fortunately, the generating function for plane partitions is known. When the result is applied to the dimer problem it will be seen that a bulk limit of the entropy does not exist.

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2. Equivalence with plane partitions

Figure 1 shows a typical dimer configuration. The dimers are placed along the edges of the lattice and are represented by double bonds. Since the maximum dimer density corresponds to each site being the endpoint of exactly one double bond, the resulting configurations are equivalent to the possible Kekulé structures of carbon–carbon bonds in graphite.

Consider now a description in terms of the dual triangular lattice. The hexagonal lattice sites are mapped into the centres of triangles; the double bonds now joining adjacent triangles in the triangular lattice. Since every triangle is joined to exactly one adjacent triangle, the dimer configuration is equivalent to a tiling of the triangular lattice with 'triangular dominoes', or rhombi (see figure 2).

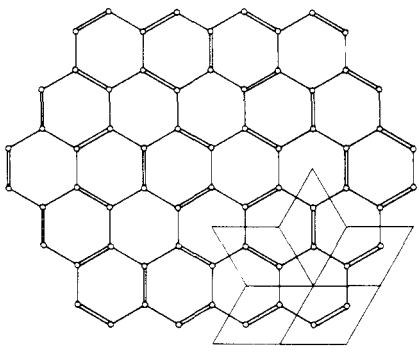

Figure 1. Dimer representation.

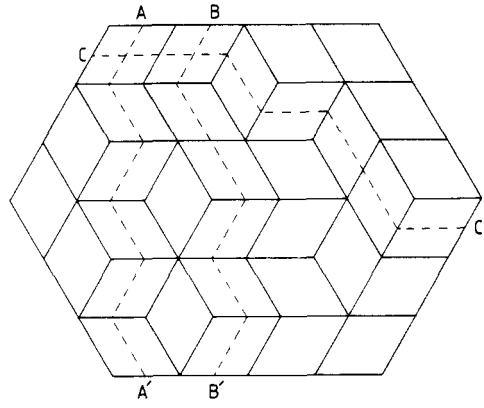

Figure 2. Tiling representation.

The tiling description will now be mapped into a three-dimensional structure. The three orientations of rhombi can be generated by projecting faces of a cube into a plane perpendicular to the cube's main diagonal. Figure 3 depicts a collection of unit cubes arranged in one octant of a three-dimensional coordinate system (portions of the planes $x = 0$, $y = 0$ and $z = 0$ are shown as well). By projecting only the 'non-hidden' surfaces of figure 3 into the (111) plane, we produce the tiling pattern of figure 2. The arrangement of unit cubes at integer points of the coordinate system follows uniquely from the tiling pattern. We proceed by building up layers of cubes. The broken line from A to A′ in figure 2 instructs us how to build up the layer for $0 < y < 1$. It consists of stacks of 3, 2 and 1 cubes in the z-direction as we proceed in the positive x-direction. The broken line AA′ is found by connecting opposite sides of the rhombi. Similarly, the layer $1 < y < 2$ is generated by following line BB′, etc. It is easy to see that the stacks of cubes always have non-increasing height as we proceed in the positive x-direction. If instead we had analysed the configuration in terms of layers of constant x (by proceeding from C to C′, etc.) we would have found that the heights of the stacks of cubes are also non-increasing in the positive y-direction. Figure 4 shows the heights of the stacks of cubes in the x–y plane. We have just shown that dimer configurations of the original hexagonal lattice correspond uniquely to the assignment of integers 0, 1, 2 or 3 to a 3×4 table such that both rows and columns form non-increasing sequences.

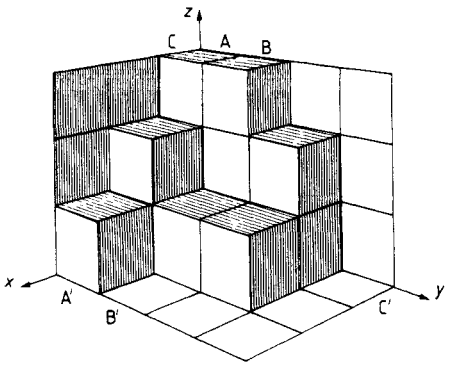

Figure 3. Three-dimensional representation.

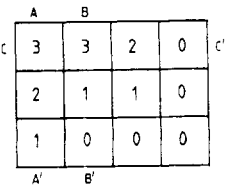

Figure 4. Plane partition.

3. The generating function

The general problem described above, of counting the number of sets of $k \times l$ integers $\{z_{ij}\}$ satisfying

$$0 \leq z_{ij} \leq m \qquad z_{ij} \leq z_{i+1\,j} \qquad z_{ij} \leq z_{ij+1}$$

is the problem of plane partitions treated extensively by MacMahon (1916). From the three-dimensional representation of figure 3 it is clear that the counting of configurations is completely symmetric with respect to permuting k, l and m. In our case, k, l and m measure the sides of the hexagon shown in figure 2. Moreover, the number of dimers belonging to the three different orientations are simply kl, lm and mk. MacMahon discovered the generating function for plane partitions:

$$G_{klm}(x) = \sum_{M=0}^{klm} P_M x^M$$

$$= \frac{F_{k+l+m}(x)F_k(x)F_l(x)F_m(x)}{F_{k+l}(x)F_{l+m}(x)F_{m+k}(x)}$$

$$F_n(x) = (1-x)^{n-1}(1-x^2)^{n-2}\ldots(1-x^{n-1}).$$

Here P_M is the number of configurations subject to the constraint

$$\sum_{\substack{1 \leq i \leq k \\ 1 \leq j \leq l}} z_{ij} = M.$$

For example,

$$G_{222}(x) = 1 + x + 3x^2 + 3x^3 + 4x^4 + 3x^5 + 3x^6 + x^7 + x^8$$

$$G_{222}(1) = 20.$$

We will evaluate G_{klm} for $x = 1$ when k, l and m are all large. Setting $x = e^{-t}$ we have,

$$\log F_n = \sum_{p=1}^{n-1} (n-p)\log(1-e^{-pt}).$$

In the limit $t \to 0$ for n large but fixed,

$$\log F_n \sim \frac{1}{t^2} \int_0^{nt} (nt-u) \log(1-e^{-u})\, du \sim \tfrac{1}{2} n^2 \log nt.$$

Substituting into the expression for G_{klm} we find:

$$S_{klm} = \log G_{klm}(1) \sim Ns(x, y, z)$$

$$N = kl + lm + mk$$

$$s(x, y, z) = \frac{1}{2(xy+yz+zx)} [x^2 \log x + y^2 \log y + z^2 \log z$$

$$-(1-x)^2 \log(1-x) - (1-y)^2 \log(1-y) - (1-z)^2 \log(1-z)]$$

$$n = k + l + m, \qquad x = k/n, \qquad y = l/n, \qquad z = m/n.$$

4. Discussion

We observe that first of all the boundary completely determines the orientational distribution of the dimers. Moreover, the specific entropy given by the function $s(x, y, z)$ is not a constant but clearly depends on the shape of the boundary. The maximum entropy per dimer is obtained when the boundary is a regular hexagon:

$$s(\tfrac{1}{3}, \tfrac{1}{3}, \tfrac{1}{3}) = \tfrac{3}{2} \log 3 - 2 \log 2 = 0.261\,6241. \tag{2}$$

Since the dimer configurations considered here are a proper subset of those counted in the toroidal problem, the entropy (2) could not have been greater than (1).

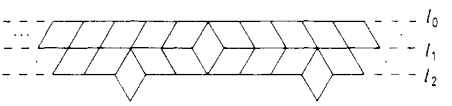

Figure 5. Hexagonal lattice.

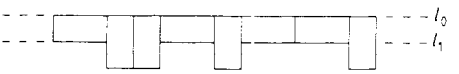

Figure 6. Square lattice.

In order to understand the difference between the square and hexagonal dimer problems when boundaries are present we focus on the nature of configurations near a single straight boundary. In figure 5, line l_0 describes the boundary and has no dimers crossing over it. Line l_1 may be crossed by at most one dimer, line l_2 by at most two, and so on. Now if at some distance away from the boundary, say near the line l_k, the dimer configurations were representative of a bulk sample, then a fixed *fraction* of l_k would be crossed by dimers. By the previous remark this requires that k be proportional to the length of the boundary. Thus the region between l_0 and l_k where the dimers are not representative of bulk properties does not become negligible when we take the thermodynamic limit. We see in figure 6 that the square lattice has a very different behaviour. Already at line l_1 the number of crossing dimers can be close to the bulk value.

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