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SOLUTION OF THE DIMER PROBLEM ON A HEXAGONAL LATTICE*

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ABSTRACT

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

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The statistical mechanics of dimers adsorbed on a crystal surface has been the subject of much theoretical work but has thus far defied solution except for the exceptional case of maximum dimer density. For the square lattice, Fisher and Temperley[1] and independently Kasteleyn[2] obtained the entropy per dimer,

$$\frac{2}{\pi}(1-\frac{1}{3^2}+\frac{1}{5^2}-\frac{1}{7^2}+\cdots)$$

using techniques involving the Pfaffian. In this note, the pure dimer problem on the hexagonal lattice will be shown to be equivalent to enumerating the "plane partitions" [3] for which a solution is already known.

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 centers 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 Fig. 2).

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

Fig. 3 into the (111) plane, we produce the tiling pattern of Fig.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 dashed line from A to A' in Fig.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 dashed line AA' is found by connecting opposite sides of the rhombi. Similarily, 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 analyzed 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.

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

$$0 \leq z_{ij} \leq m$$

$$z_{ij} \leq z_{i+1j}$$

$$z_{ij} \leq z_{ij+1}$$

is the problem of plane partitions treated extensively by MacMahon[3]. From the three-dimensional representation of Fig.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 Fig.2. Moreover, the number of dimers belonging to the three different orientations are simply $k \cdot l$, $l \cdot m$ and $m \cdot k$. MacMahon discovered the generating function for plane partitions:

$$G_{klm}(x) = \sum_{N=0}^{klm} P_N x^N$$
$$= \frac{F_{k+l+m}(x)F_k(x)F_l(x)F_m(x)}{F_{k+l}(x)F_{l+m}(x)F_{m+k}(x)}$$

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

Here P_N is the number of configurations subject to the constraint,

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

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,

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

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

$$S_{klm} = \log G_{klm}(1)$$
$$\sim \frac{1}{2}n^2[x^2\log x + y^2\log y + z^2\log z$$
$$-(1-x)^2\log(1-x) - (1-y)^2\log(1-y) - (1-z)^2\log(1-z)]$$

$$n = k + l + m, \quad x = \frac{k}{n}, \quad y = \frac{l}{n}, \quad z = \frac{m}{n}$$

If a bulk limit of the entropy had existed we would have obtained a constant multiple of $kl + lm + mk$.

Unlike the square lattice problem (with similar boundary conditions) here the boundary determines the orientational distribution of the dimers. However, once we consider the general monomer-dimer system with non-zero monomer density ρ, this constraint no longer applies. Thus, whereas a bulk limit of the entropy does not exist for the case $\rho = 0$, such a limit may exist for the case $\rho \to 0$.

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References

[1] Temperley, H.N.V., and M.E.Fisher, *Phil.Mag.* **6**, *1061* (1961)

Fisher, M.E., *Phys.Rev.* **124**, *1664* (1961)

[2] Kasteleyn, P.W., *Physica* **27**, *1209* (1961)

[3] MacMahon, P.A., **Combinatory Analysis** vol.2, Cambridge University Press 1916

Chaundy, T.W., *Quart.Jour.Math.* **2**, *234* (1931)

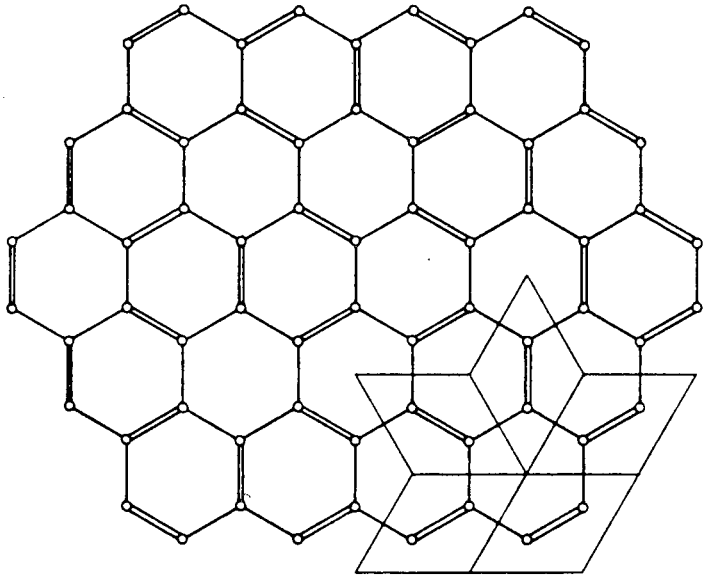

Figure 1

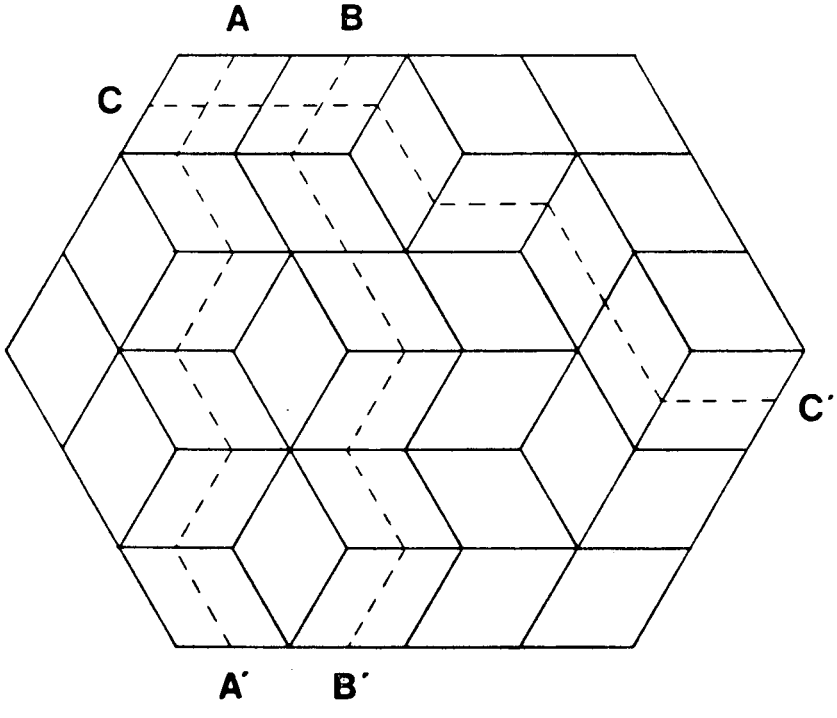

Figure 2

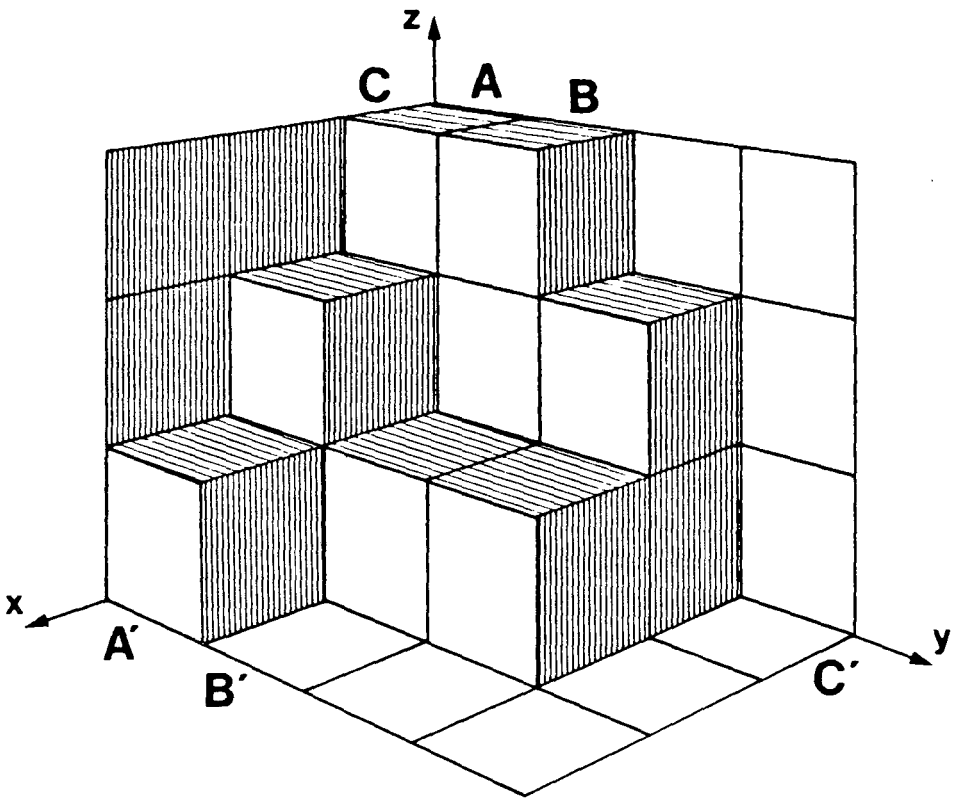

Figure 3

	A	B		
C	3	3	2	0	C′
	2	1	1	0	
	1	0	0	0	
	A′	B′		

Figure 4

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