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A note on the monomer dimer problem

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In this note we determine a lower bound for the number of different configurations of monomers and dimers on the hypercubical lattice. This combinatorial problem has important applications in statistical mechanics ((1)) and solid state chemistry.

Statement of the problem and principal results. Denote by $A(n,d)$ the set of sites of the d-dimensional hypercubical lattice having integer coordinates $(x_1, x_2, \ldots, x_d)$ where for each $i\,(0 \leqslant x_i \leqslant n-1)$. A *monomer* is a single atom and a *dimer* consists of two atoms joined by a bond of unit length. Let $f(n,d;s)$ denote the number of ways in which the sites of $A(n,d)$ may be completely covered by s dimers and $(n^d - 2s)$ monomers.

Hammersley ((2)) has proved that there exists a continuous concave function $\lambda_d(p)$ such that as $n \to \infty$ and $2s/n \to p$

$$\lim_{n\to\infty} n^{-d} \log f(n,d;s) = \lambda_d(p) \tag{1}$$

and that for $d > 1$ $$\lambda_d(p) \leqslant \alpha_d(p) = (\tfrac{1}{2}p)\log d + \lambda_1(p). \tag{2}$$

It is easy to show that

$$\lambda_1(p) = (1-\tfrac{1}{2}p)\log(1-\tfrac{1}{2}p) - (\tfrac{1}{2}p)\log(\tfrac{1}{2}p) - (1-p)\log(1-p) \tag{3}$$

and that $$\lambda_d(p) \leqslant \lambda_{d+1}(p) \quad (d \geqslant 1) \tag{4}$$

and Hammersley ((2)) uses the concavity of $\lambda_d(p)$ to combine (4) with the result

$$\lambda_d(p) \geqslant \lambda_d(1) - (\tfrac{1}{2}p)\log p - \tfrac{1}{2}(1-p)\log(2d(1-p)). \tag{5}$$

This, however, is a weak lower bound, particularly for $d > 2$. In this note we prove that if $0 \leqslant p \leqslant 2d/(4d-1)$

$$\lambda_d(p) \geqslant \frac{p}{2}\log\left(\frac{2d-p(4d-1)}{p}\right) + \frac{d}{4d-1}\log\left(\frac{2d}{2d-p(4d-1)}\right) \tag{6}$$

and if $(4d-2)/(4d-1) \leqslant p \leqslant 1$ then

$$\lambda_d(p) \geqslant \lambda_d(1) + \left(\frac{1-p}{2}\right)\log\left(\frac{1-(4d-1)(1-p)}{1-p}\right) - \frac{1}{2(4d-1)}\log(1-(4d-1)(1-p)). \tag{7}$$

The result (7) clearly depends strongly on $\lambda_d(1)$. Fisher ((3)) and Kasteleyn ((4)) have proved independently that

$$\lambda_2(1) = 0{\cdot}29156090\ldots, \tag{8}$$

but have not been able to extend their results to higher dimensions.

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In a private communication M. E. Fisher has shown that

$$\lambda_3(1) \geqslant 0{\cdot}30187 \tag{9}$$

and from (2)

$$\lambda_3(1) \leqslant 0{\cdot}5493, \tag{10}$$

but these are very weak results. Fisher indeed conjectures that $\lambda_3(1)$ is approximately 0·43.

In the table below we compare the bounds obtained for $\lambda_d(p)$ for $d = 2$ and 3. $\beta_d(p)$ denotes the lower bound obtained by combining (6) and (7) by concavity, and using (8) and (9).

P	$\lambda_1(p)$	$\beta_2(p)$	$\alpha_2(p)$	$\beta_3(p)$	$\alpha_3(p)$
0·1	0·1959	0·2298	0·2306	0·2498	0·2508
0·2	0·3140	0·3796	0·3833	0·4190	0·4339
0·3	0·3961	0·4895	0·5001	0·5474	0·5609
0·4	0·4492	0·5637	0·5878	0·6377	0·6689
0·5	0·4774	0·5941	0·6507	0·6777	0·7521
0·6	0·4780	0·5537	0·6859	0·6175	0·8076
0·7	0·4486	0·5133	0·6912	0·5573	0·8331
0·8	0·3823	0·4729	0·6595	0·4971	0·8217
0·9	0·2607	0·4325	0·5726	0·4369	0·7551
1·0	0·0000	0·2916	0·2916	0·3019	0·5493

Proof of result (6). The number of configurations in which the sites $A(n, d)$ are covered by $(n^d - 2)$ monomers and a single dimer is clearly

$$f(n, d;\ 1) = d(n-1)\, n^{d-1}.$$

If P_1 and P_2 are the adjacent sites of $A(n, d)$ occupied by this single dimer, a second dimer can be placed anywhere in the lattice provided it does not join either P_1 or P_2 to its nearest neighbours in the lattice. Thus a second dimer has at least $f(n, d;\ 1) - (4d-1)$ possible positions in $A(n, d)$. Hence

$$f(n, d;\ 2) \geqslant \frac{f(n, d;\ 1)\,(f(n, d;\ 1) - 4d + 1)}{2!},$$

and in general if there are k dimers in position on the sites $\{P_i, 1 \leqslant i \leqslant 2k\}$ of $A(n, d)$, a $(k+1)$th dimer cannot be placed so that either of its end-points coincides with any P_i. Hence the $(k+1)$th dimer has at least $f(n, d;\ 1) - k(4d-1)$ possible positions in $A(n, d)$. Thus provided

$$f(n, d;\ 1) - (s-1)\,(4d-1) \geqslant 0 \tag{11}$$

we have

$$f(n, d;\ s) \geqslant (s!)^{-1} \prod_{k=0}^{s-1} (f(n, d;\ 1) - k(4d-1))$$

which implies

$$f(n, d;\ s) \geqslant (4d-1)^s \binom{A}{s}, \tag{12}$$

where

$$A = [f(n, d;\ 1)/(4d-1)] = [d(n-1)\, n^{d-1}/(4d-1)].$$

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If we now let $n \to \infty$ and $2s/n^d \to p$ a straightforward application of Stirling's formula gives the result (6), provided that by (11)

$$0 \leqslant p \leqslant 2d/(4d-1).$$

Proof of result (7). Let n be even. Denote by $\Omega(n, s)$ the set of distinct coverings of $A(n, d)$ by s dimers and $(n^d - 2s)$ monomers. Given a member $w_0 \in \Omega(n, \frac{1}{2}n^d)$ we successively replace k dimers of w_0 by $2k$ monomers, obeying the rule that at each stage the selected dimer must not have an end-point at any site which has as a nearest neighbour a monomer already in the configuration. In this way we arrive at a configuration $w_0(k) \in \Omega(n, \frac{1}{2}n^d - k)$ and moreover if $w_1 \in \Omega(n, \frac{1}{2}n^d)$ and $w_1 \neq w_0$ then it is easy to see that the configuration $w_0(k)$ cannot be derived from w_1 by applying the above rule.

The number of distinct configurations in $\Omega(n, \frac{1}{2}n^d - k)$ which may be derived from a fixed $w_0 \in \Omega(n, \frac{1}{2}n^d)$ is clearly not less than

$$g(d, n, k) = (k!)^{-1} \prod_{r=0}^{k-1} \left(\frac{n^d}{2} - r(4d-1) \right)$$

provided $$\tfrac{1}{2}n^d - (4d-1)(k-1) \geqslant 0. \tag{13}$$

If $B = [n^d/2(4d-1)]$ $$g(d, n, k) = (4d-1)^k \binom{B}{k}$$

and hence provided (13) is satisfied

$$f(n, d; (\tfrac{1}{2}n^d) - k) \geqslant f(n, d; \tfrac{1}{2}n^d)(4d-1)^k \binom{B}{k}. \tag{14}$$

If we now let $n \to \infty$ in such a way that $2(\frac{1}{2}n^d - k)/n^d \to p$ we get the required result (7) by applying Stirling's formula and (1) to the inequality (14), where the range of p is determined by (13).

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