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An improved lower bound for the multidimensional dimer problem

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1. *Introduction.* The dimer problem, which in the three-dimensional case is one of the classical unsolved problems of solid-state chemistry, can be formulated mathematically as follows. We define a *brick* to be a d-dimensional ($d \geqslant 2$) rectangular parallelopiped with sides whose lengths are integers. An *n-brick* is a brick whose volume is n; and a dimer is a 2-brick. The problem is to determine the number of ways of dissecting an n-brick into dimers; and since this is only possible when n is even we confine attention hereafter to n-bricks with n even. Consider an n-brick with sides of length $a_1, a_2, \ldots, a_d$, where $n = a_1 a_2 \ldots a_d$, and write $\mathbf{a} = (a_1, a_2, \ldots, a_d)$. Let $f_{\mathbf{a}}$ denote the number of ways of dissecting this brick into $\frac{1}{2}n$ dimers. On the basis of physical and heuristic arguments chemists have known for many years that $f_{\mathbf{a}}$ increases more or less exponentially with n; and recently a rigorous proof (1) of this fact has been given in the following form: if $a_i \to \infty$ for all $i = 1, 2, \ldots, d$, then $n^{-1} \log f_{\mathbf{a}}$ tends to a finite limit, which we denote by λ_d. The principal outstanding problem for chemists is to determine the numerical value of λ_3, or failing an exact determination to estimate λ_3 or to find upper and lower bounds for it.

There is an extensive literature to this problem, with a variety of approximations to λ_2 and λ_3, some good and some bad. The celebrated early paper by Fowler and Rushbrooke (2) gave the estimate $\lambda_2 = 0{\cdot}29$ and $\lambda_3 = 0{\cdot}43$ together with the rigorous bounds

$$0 \leqslant \lambda_d \leqslant \tfrac{1}{2} \log d. \tag{1}$$

Many years later, Hurst and Green(3) showed that the two-dimensional Ising problem could be resolved by using anti-commuting matrices and Pfaffians; and this idea was then adapted to the two-dimensional dimer problem by Fisher, Kasteleyn and Temperley (each working independently of the other two), who found that

$$\lambda_2 = \frac{1}{\pi} \sum_{r=0}^{\infty} \frac{(-1)^r}{(2r+1)^2} = 0{\cdot}29156090\ldots \tag{2}$$

Temperley and Fisher(4) published a joint announcement of this result; and Fisher (5) and Kastelyn (6, 7) published proofs of it.

Since λ_d is clearly a non-decreasing function of d, (1) and (2) yield

$$0{\cdot}29156 \leqslant \lambda_3 \leqslant 0{\cdot}54931. \tag{3}$$

According to Bondy and Welsh (8), Fisher (in a private communication which I have not seen) has proved the sharper result

$$0{\cdot}30187 \leqslant \lambda_3 \tag{4}$$

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and has conjectured that λ_3 is approximately 0·43. As far as I know, (4) is the best rigorous lower bound hitherto obtained for λ_3. The Fowler–Rushbrooke estimate of $\lambda_3 = 0{\cdot}43$ must command a good deal of respect in view of their successful prediction of the value of λ_2. Rushbrooke, in a private communication to Nagle (9), revised his estimate to $\lambda_3 = 0{\cdot}45$. Some other estimates close to this value are $\lambda_3 = 0{\cdot}4400$, due to Miller (10) and Chang (11), and $\lambda_3 = 0{\cdot}44641$ and $\lambda_3 = 0{\cdot}44647$ resulting from two different techniques exploited by Nagle (9).

The main result of the present paper is the rigorous lower bound

$$0{\cdot}418347 \leqslant \lambda_3. \tag{5}$$

This is a particular case of the more general result

$$\lambda_d \geqslant \frac{1}{4\pi^d}\int_0^\pi d\theta_1 \int_0^\pi d\theta_2 \ldots \int_0^\pi d\theta_d \log\left\{4\sum_{i=1}^{d}\sin^2\theta_i\right\} \tag{6}$$

which I shall also prove. In proving (6), I shall find an exact expression for $f_{\mathfrak{a}}$ in terms of a permanent. The relevance of permanents to this problem is mentioned very briefly by Kasteleyn (7) and also by Caianiello (12). As will be shown presently, a permanent arises naturally in this kind of problem as a result of a combinatorial theorem (13) on systems of distinct representatives. It is interesting to compare this approach by way of permanents with the alternative (but less direct) technique based on sets of anti-commuting matrices (5).

2. *Proof of results.* If $\mathbf{V} = (v_{ij})$ is an $n \times n$ matrix, the permanent of $\mathbf{V}$ is defined to be

$$\text{per } \mathbf{V} = \Sigma_\pi v_{1\pi(1)} v_{2\pi(2)} \ldots v_{n\pi(n)}, \tag{7}$$

where the sum is taken over all permutations $\pi(1), \pi(2), \ldots, \pi(n)$ of the set $1, 2, \ldots, n$. Let S be a finite set with elements $e_1, e_2, \ldots, e_n$; and let $S_1, S_2, \ldots, S_n$ be given subsets of S. If we can find a permutation $\pi(1), \pi(2), \ldots, \pi(n)$ such that $e_{\pi(i)} \in S_i$ for $i = 1, 2, \ldots, n$, then the ordered set $\{e_{\pi(1)}, e_{\pi(2)}, \ldots, e_{\pi(n)}\}$ is called a *system of distinct representatives* of $S_1, S_2, \ldots, S_n$. We shall use the following theorem ((13), p. 54): *the number of different systems of distinct representatives* of $S_1, S_2, \ldots, S_n$ *is* per $\mathbf{V}$, *where* $v_{ij} = 0$ *or* 1 *according as* e_j *does not or does belong to* S_i. The theorem is very easily proved: indeed the proof is no more than a matter of inspection, because each product in the sum (7) is 1 or 0 according as $\{e_{\pi(1)}, e_{\pi(2)}, \ldots, e_{\pi(n)}\}$ is or is not a system of distinct representatives.

Now consider the n-brick with sides $a_1, a_2, \ldots, a_d$. This is the union of n unit cubes, which we may imagine to be coloured alternately black and white after the fashion of a chessboard: that is to say those cubes, which facially abut a given cube, are all of opposite colour to the given cube. We call these facially abutting cubes the *neighbours* of the given cube. Let $e_1, e_2, \ldots, e_n$ be a fixed enumeration of the n cubes which compose the n-brick; and let S_i be the set of neighbours of e_i. S_i will usually consist of $2d$ cubes, although S_i will contain fewer cubes than this if e_i lies on the surface or at a corner of the n-brick. The matrix $\mathbf{V}$, defined in the previous paragraph, will simply be the incidence matrix of the set of cubes: that is to say $v_{ij} = 0$ or 1 according as e_i and e_j do not or do abut facially.

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Suppose that $\{e_{\pi(1)}, e_{\pi(2)}, \ldots, e_{\pi(n)}\}$ is a given system of distinct representatives of $S_1, S_2, \ldots, S_n$. If e_i is a black cube, we place a black dimer on the adjacent cubes e_i and $e_{\pi(i)}$; while if e_i is a white cube, we place a white dimer on the adjacent cubes e_i and $e_{\pi(i)}$. Consider the complete set of white dimers thus positioned. The n-brick contains $\frac{1}{2}n$ white cubes; so there are $\frac{1}{2}n$ white dimers in the set. Each white dimer covers one white cube and one black cube; so the set of white dimers covers the white cubes in the set $\{e_1, e_2, \ldots, e_n\}$ and the black cubes in the set $\{e_{\pi(1)}, e_{\pi(2)}, \ldots, e_{\pi(n)}\}$. Since the cubes of $\{e_1, e_2, \ldots, e_n\}$ are all distinct, and since the cubes of $\{e_{\pi(1)}, e_{\pi(2)}, \ldots, e_{\pi(n)}\}$ are all distinct, and since no cube is both black and white, the number of cubes covered by the white dimers is n. Therefore the white dimers constitute a dissection of the n-brick into $\frac{1}{2}n$ dimers. Similarly the black dimers constitute another dissection of the n-brick into $\frac{1}{2}n$ dimers. Thus the system of distinct representatives $\{e_{\pi(1)}, e_{\pi(2)}, \ldots, e_{\pi(n)}\}$ specifies a pair of dissections of the n-brick into dimers. Conversely, suppose that we are given any pair of dissections of the n-brick. We let the first dissection be a dissection into white dimers, and the second dissection a dissection into black dimers. If the cube e_i is white, let $e_{\pi(i)}$ be the black cube which lies at the other end of the white dimer covering e_i; while if e_i is black, let $e_{\pi(i)}$ be the white cube which lies at the other end of the black dimer covering e_i. Then, as before, the elements in the set $\{e_{\pi(1)}, e_{\pi(2)}, \ldots, e_{\pi(n)}\}$ are all distinct and respectively belong to $S_1, S_2, \ldots, S_n$.

The foregoing argument shows that there is a (1, 1)-correspondence between pairs of dissections and systems of distinct representatives. The number of pairs of dissections is obviously $f_{\mathbf{a}}^2$. Hence, by the theorem on the number of different systems of distinct representatives, we get

$$f_{\mathbf{a}}^2 = \operatorname{per} \mathbf{V}, \tag{8}$$

where $\mathbf{V}$ is the incidence matrix of neighbouring cubes. Since it is easy to write down $\mathbf{V}$ we have reduced the dimer problem to the problem of evaluating a permanent. Unfortunately, there is no known convenient method of evaluating a permanent.

Since it is much easier to evaluate a determinant than a permanent, let us compare (7) with the expression for the determinant of a matrix $\mathbf{U} = (u_{ij})$, namely

$$\det \mathbf{U} = \Sigma_\pi \delta_\pi u_{1\pi(1)} u_{2\pi(2)} \ldots u_{n\pi(n)}, \tag{9}$$

where $\delta_\pi = +1$ or -1 according as the permutation $\pi(1), \pi(2), \ldots, \pi(n)$ is even or odd. Suppose that U is *any* real matrix such that $|u_{ij}| = v_{ij}$, that is to say the elements of $\mathbf{U}$ and $\mathbf{V}$ agree apart from sign. Since every term in (7) is non-negative when $\mathbf{V}$ is an incidence matrix, we have $\operatorname{per} \mathbf{V} \geqslant \det \mathbf{U}$ and hence, by (8)

$$f_{\mathbf{a}}^2 \geqslant \det \mathbf{U}. \tag{10}$$

We may, and shall, use (10) to obtain a lower bound for λ_d.

At this stage the question naturally crops up of whether we might perhaps be able to choose the signs of the elements u_{ij} such that every term in the expansion (9) is non-negative; for if we could do this then equality would hold in (10), and we should have reduced the dimer problem to the fairly simple problem of evaluating a determinant. This is in fact possible when $d = 2$. I do not know whether it is also possible for $d > 2$; though the work of Tinsley (14) on somewhat related matters suggests that the prospects

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are not too hopeful. In passing it is worth mentioning that, although we specified above that $\mathbf{U}$ should be a real matrix, there is no compelling reason for this. Indeed if $\mathbf{U}$ is a complex matrix such that $|u_{ij}| = v_{ij}$, then

$$f_{\mathbf{a}}^2 \geqslant |\det \mathbf{U}|, \tag{11}$$

and (11) might turn out to be a sharper inequality than (10) for a suitable complex $\mathbf{U}$.

Before going further, let us compare what we have so far done with Fisher's treatment for $d = 2$. He starts off from a system of anti-commuting matrices, and expresses $f_{\mathbf{a}}$ as the trace of a polynomial in these matrices. He next invokes a theorem which expresses this trace as a Pfaffian, and then Cayley's theorem which asserts that the square of a Pfaffian equals the determinant of a skew-systematic matrix. Thus $f_{\mathbf{a}}^2 = \det \mathbf{U}$, where $\mathbf{U}$ is this skew-symmetric matrix; and it turns out that the elements of $\mathbf{U}$ are those of $\mathbf{V}$ apart from sign. The point of interest here is the way in which the square of $f_{\mathbf{a}}$ arises in the two approaches: namely, by way of Cayley's theorem in Fisher's approach, and in the present treatment by way of the $(1, 1)$ correspondence between *pairs* of dissections and systems of distinct representatives.

In a moment we shall write down the incidence matrix $\mathbf{V}$ for a brick. It is, however, worth remarking that we could equally well write down the incidence matrix for a toroidal brick, obtained by identifying and joining opposite faces of the original brick. For this the incidence matrix $\mathbf{V}^*$ would be a circulant matrix, and this might perhaps offer certain advantages: for example it would fall more within the ambit of Tinsley's researches (14). If $f_{\mathbf{a}}^*$ were the number of dimer dissections of a toroidal brick, we should get

$$f_{\mathbf{a}}^2 \leqslant f^{*2} = \operatorname{per} \mathbf{V}^*; \tag{12}$$

but we could still use this to find bounds for λ_d (or conceivably even determine λ_d exactly) since it is not hard to prove by a fairly straightforward variant of the analysis in (1) that $n^{-1} \log f_{\mathbf{a}}^*$ also converges to λ_d as $a_i \to \infty$ for each $i = 1, 2, \ldots, d$. But the prospects of this line of attack are not at all clear to me, and I shall not pursue it further in this paper.

Since $n^{-1} \log f_{\mathbf{a}} \to \lambda_d$ for any $a_i \to \infty$, we may as well simplify the argument by choosing the a_i all equal, in which case they must all be even since n is even. Thus write $a_i = 2b$ for $i = 1, 2, \ldots, d$ and $n = (2b)^d$.

We may number the cubes $e_1, e_2, \ldots, e_n$ in any way we please; and we choose the method which directly generalizes Fisher's approach for the case $d = 2$. When $d = 2$ the cubes become squares of a chessboard; and Fisher numbered them in boustrephedon fashion: that is to say, he numbered them from e_1 to e_n along a path which started with e_1 at the top left-hand corner of the chessboard, ran along the top row from left to right, then along the second row from right to left, and so on from left to right and from right to left in alternate rows until the bottom left-hand corner was reached at e_n. For $d > 2$, we can imagine a d-dimensional chessboard made up of $2b$ layers, each layer being a $(d-1)$-dimensional chessboard. Suppose that we know how to construct a boustrephedon path for a $(d-1)$-dimensional board. Then we can construct a boustrephedon path for a d-dimensional board as follows. Start with the top layer and number the cubes in this layer by a $(d-1)$-dimensional boustrephedon path. Then

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descend from the last cube of the top layer to the cube immediately below it in the second layer, and then follow in the second layer a boustrephedon path which is exactly the same as the path in the top layer except that it is described in the opposite direction. Subsequently proceed to successively lower layers in which the same path is described forwards and backwards in alternate layers until the bottom layer is dealt with. It is quite easy to see that, if $\mathbf{V}_d$ is the incidence matrix for a boustrephedon enumeration of a d-dimensional brick, then $\mathbf{V}_d$ will be a matrix of the order $(2b)^d$ which can be written in the following partitioned form

$$\mathbf{V}_d = \begin{pmatrix} \mathbf{V}_{d-1} & \mathbf{J}_{d-1} & \mathbf{0} & \mathbf{0} & \dots & \mathbf{0} \\ \mathbf{J}_{d-1} & \mathbf{V}_{d-1} & \mathbf{J}_{d-1} & \mathbf{0} & \dots & \mathbf{0} \\ \mathbf{0} & \mathbf{J}_{d-1} & \mathbf{V}_{d-1} & \mathbf{J}_{d-1} & \dots & \mathbf{0} \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \dots & \mathbf{V}_{d-1} \end{pmatrix}, \tag{13}$$

where $\mathbf{J}_{d-1}$ is the matrix obtained by reversing the order of the columns of a unit matrix of order $(2b)^{d-1}$, and $\mathbf{0}$ is a zero matrix of order $(2b)^{d-1}$. In (13) there are $2b$ rows and $2b$ columns of submatrices. The recursion involved in (13) starts from the matrix

$$\mathbf{V}_1 = \begin{pmatrix} 0 & 1 & 0 & \dots & 0 & 0 \\ 1 & 0 & 1 & \dots & 0 & 0 \\ 0 & 1 & 0 & \dots & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \dots & 1 & 0 \end{pmatrix} \tag{14}$$

of order $2b$.

In forming $\mathbf{U}$ from $\mathbf{V}$ we may adjust the signs of the elements in $\mathbf{V}$ in any way we please; and, following Fisher's lead for the case $d = 2$, we choose $\mathbf{U}$ to be the skew-symmetric matrix which coincides with $\mathbf{V}$ on and above the principal diagonal. Thus $\mathbf{U} = \mathbf{U}_d$ where

$$\mathbf{U}_d = \begin{pmatrix} \mathbf{U}_{d-1} & \mathbf{J}_{d-1} & \mathbf{0} & \mathbf{0} & \dots & \mathbf{0} \\ -\mathbf{J}_{d-1} & \mathbf{U}_{d-1} & \mathbf{J}_{d-1} & \mathbf{0} & \dots & \mathbf{0} \\ \mathbf{0} & -\mathbf{J}_{d-1} & \mathbf{U}_{d-1} & \mathbf{J}_{d-1} & \dots & \mathbf{0} \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \dots & \mathbf{U}_{d-1} \end{pmatrix}. \tag{15}$$

Instead of starting the recurrence from $\mathbf{U}_1$, the skew-symmetric form of $\mathbf{V}_1$, it is more convenient to start it from $\mathbf{U}_0$, defined to be the zero matrix of order 1. Thus (15) is to hold for all $d \geqslant 1$, and of course $\mathbf{J}_0$ will simply be the unit matrix of order 1.

We now proceed to evaluate $\det \mathbf{U}_d$. It is simpler to proceed indirectly by evaluating instead $\det(\mathbf{U}_d^2) = (\det \mathbf{U}_d)^2$. It is easy to see that, if we reverse both the order of rows and the order of the columns in $\mathbf{U}_d$, then $\mathbf{U}_d$ becomes $-\mathbf{U}_d$ provided this is true for $\mathbf{U}_{d-1}$; but it is obviously true for $\mathbf{U}_1$, and therefore for $\mathbf{U}_d$ by induction. Since reversal

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of the order of rows and of columns is achieved by premultiplying and postmultiplying by $\mathbf{J}_d$, we have

$$\mathbf{J}_d\mathbf{U}_d\mathbf{J}_d = -\mathbf{U}_d \quad (d \geqslant 0). \tag{16}$$

Also

$$\mathbf{J}_d^2 = \mathbf{I}_d \quad (d \geqslant 0), \tag{17}$$

where $\mathbf{I}_d$ is the unit matrix of order $(2b)^d$. Hence

$$\mathbf{J}_d\mathbf{U}_d = -\mathbf{U}_d\mathbf{J}_d \quad (d \geqslant 0). \tag{18}$$

From (15), (17), and (18) we find for any scalar λ,

$$\mathbf{U}_d^2 - \lambda\mathbf{I}_d = \begin{pmatrix} \mathbf{P} & 0 & \mathbf{I} & 0 & 0 & \dots & 0 & 0 & 0 \\ 0 & \mathbf{R} & 0 & \mathbf{I} & 0 & \dots & 0 & 0 & 0 \\ \mathbf{I} & 0 & \mathbf{R} & 0 & \mathbf{I} & \dots & 0 & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & 0 & 0 & \dots & \mathbf{I} & 0 & \mathbf{P} \end{pmatrix}, \tag{19}$$

where $\mathbf{I} = \mathbf{I}_{d-1}$ and all elements on the principal diagonal are $\mathbf{R} = \mathbf{U}_{d-1}^2 - (2+\lambda)\mathbf{I}_{d-1}$ except the first and the last which are $\mathbf{P} = \mathbf{U}_{d-1}^2 - (1+\lambda)\mathbf{I}_{d-1}$. Now rearrange the rows of submatrices on the right-hand side of (19) so that first come the odd-numbered rows in their normal order, followed by the even-numbered rows in reverse order; and rearrange the columns similarly. The right-hand side then takes the form

$$\begin{pmatrix} \mathbf{X} & 0 \\ 0 & \mathbf{X} \end{pmatrix},$$

where

$$\mathbf{X} = \begin{pmatrix} \mathbf{P} & \mathbf{I} & 0 & \dots & 0 \\ \mathbf{I} & \mathbf{R} & \mathbf{I} & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \dots & \mathbf{R} \end{pmatrix} \tag{20}$$

in which all diagonal elements except the first are $\mathbf{R}$. Consequently

$$\det(\mathbf{U}_d^2 - \lambda\mathbf{I}_d) = \pm(\det\mathbf{X})^2,$$

and we must choose the positive sign, since this choice of sign depends only on a fixed rearrangement of rows and columns and so is independent of λ, and the left-hand side is $(\det\mathbf{U}_d)^2$ when $\lambda = 0$. Thus

$$\det(\mathbf{U}_d^2 - \lambda\mathbf{I}_d) = (\det\mathbf{X})^2. \tag{21}$$

Now consider the functions

$$g_r = g_r(x) = \cos r\theta + \cot\theta \sin r\theta \quad (r = 0, 1, 2, \dots), \tag{22}$$

where $x = -2\cos\theta$. It is easy to verify from (22) that

$$g_0 = 1, \quad g_1 = -x, \quad g_r + xg_{r-1} + g_{r-2} = 0 \quad (r \geqslant 2); \tag{23}$$

and hence $g_r(x)$ is a polynomial in x of degree r. Let $\mathbf{G}_r$ be the corresponding polynomial in the matrix $\mathbf{R}$; so that

$$\mathbf{G}_0 = \mathbf{I}, \quad \mathbf{G}_1 = -\mathbf{R}, \quad \mathbf{G}_r + \mathbf{R}\mathbf{G}_{r-1} + \mathbf{G}_{r-2} = 0 \quad (r \geqslant 2). \tag{24}$$

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In view of (24) we have

$$\begin{pmatrix} \mathbf{G}_0 & \mathbf{G}_1 & \mathbf{G}_2 & \dots & \mathbf{G}_{b-1} \\ \mathbf{0} & \mathbf{G}_0 & \mathbf{G}_1 & \dots & \mathbf{G}_{b-2} \\ \mathbf{0} & \mathbf{0} & \mathbf{G}_0 & \dots & \mathbf{G}_{b-3} \\ \dots & \dots & \dots & \dots & \dots \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \dots & \mathbf{G}_0 \end{pmatrix} \begin{pmatrix} \mathbf{R}+\mathbf{I} & \mathbf{I} & \mathbf{0} & \dots & \mathbf{0} & \mathbf{0} \\ \mathbf{I} & \mathbf{R} & \mathbf{I} & \dots & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} & \mathbf{R} & \dots & \mathbf{0} & \mathbf{0} \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \dots & \mathbf{I} & \mathbf{R} \end{pmatrix}$$

$$= \begin{pmatrix} \mathbf{I} & \mathbf{0} & \mathbf{0} & \dots & \mathbf{0} & -\mathbf{G}_b \\ \mathbf{I} & \mathbf{0} & \mathbf{0} & \dots & \mathbf{0} & -\mathbf{G}_{b-1} \\ \mathbf{0} & \mathbf{I} & \mathbf{0} & \dots & \mathbf{0} & -\mathbf{G}_{b-2} \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \dots & \mathbf{I} & -\mathbf{G}_1 \end{pmatrix}. \tag{25}$$

The first matrix in (25) has unit determinant, since $\mathbf{G}_0 = \mathbf{I}$; the second matrix is $\mathbf{X}$, since $\mathbf{P} = \mathbf{R}+\mathbf{I}$; and the third matrix has determinant $\pm\det(\mathbf{G}_b - \mathbf{G}_{b-1})$. Hence (21) and (25) yield

$$\det(\mathbf{U}_d^2 - \lambda\mathbf{I}_d) = [\det(\mathbf{G}_b - \mathbf{G}_{b-1})]^2. \tag{26}$$

From (22), we obtain after a little manipulation

$$g_b(x) - g_{b-1}(x) = -\sec\tfrac{1}{2}\theta\cos(b+\tfrac{1}{2})\theta, \tag{27}$$

which vanishes when

$$\theta = (m+\tfrac{1}{2})\pi/(b+\tfrac{1}{2}) \quad (m = 0, 1, \dots, b-1). \tag{28}$$

Since $x = -2\cos\theta$, we get from (27) and (28)

$$g_b(x) - g_{b-1}(x) = \prod_{m=0}^{b-1}\left(x + 2\cos\frac{m+\frac{1}{2}}{b+\frac{1}{2}}\pi\right) \tag{29}$$

and therefore

$$\begin{aligned} \mathbf{G}_b - \mathbf{G}_{b-1} &= \prod_{m=0}^{b-1}\left(\mathbf{R} + 2\mathbf{I}\cos\frac{m+\frac{1}{2}}{b+\frac{1}{2}}\pi\right) \\ &= \prod_{m=0}^{b-1}\left\{\mathbf{U}_{d-1}^2 - \left(\lambda + 2 - 2\cos\frac{m+\frac{1}{2}}{b+\frac{1}{2}}\pi\right)\mathbf{I}_{d-1}\right\} \\ &= \prod_{m=0}^{b-1}\left\{\mathbf{U}_{d-1}^2 - \left(\lambda + 4\sin^2\frac{m+\frac{1}{2}}{2b+1}\pi\right)\mathbf{I}_{d-1}\right\}. \end{aligned} \tag{30}$$

The last expression in (30) is unchanged if we take the product over $m = b+1, b+2, \dots, a$ instead of $m = 0, 1, \dots, b-1$. To this end we shall write $\prod_{m=0}^{a\neq b}$ for a product taken over all $m = 0, 1, \dots, a$ except $m = b$; and we employ a similar notation for sums in (34) below. Thus, since there is a square on the right-hand side of (26) and since $a = 2b$, we get

$$\det(\mathbf{U}_d^2 - \lambda\mathbf{I}_d) = \prod_{m=0}^{a\neq b}\det\left\{\mathbf{U}_{d-1}^2 - \left(\lambda + 4\sin^2\frac{m+\frac{1}{2}}{a+1}\pi\right)\mathbf{I}_{d-1}\right\}. \tag{31}$$

In (31) λ is an arbitrary scalar. Thus by adjusting the value of λ appropriately we can use (31) as a recurrence relation over d for expressing $\det(\mathbf{U}_d^2 - \lambda\mathbf{I}_d)$ as a product of

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terms of the form $\det(\mathbf{U}_0^2 - \mu\mathbf{I}_0) = -\mu$ since $\mathbf{U}_0$ and $\mathbf{I}_0$ are the zero and unit matrices of order 1. We find

$$\det \mathbf{U}_a^2 = \prod_{m_1=0}^{a+b} \prod_{m_2=0}^{a+b} \dots \prod_{m_d=0}^{a+b} \left\{ -4 \sum_{i=1}^{d} \sin^2 \frac{m_i + \frac{1}{2}}{a+1} \pi \right\}. \tag{32}$$

There are an even number of terms in this product, and so we may write 4 for -4 in (32). From (10) and (32) we deduce

$$f_a^4 \geqslant \prod_{m_1=0}^{a+b} \prod_{m_2=0}^{a+b} \dots \prod_{m_d=0}^{a+b} \left\{ 4 \sum_{i=1}^{d} \sin^2 \frac{(m_i + \frac{1}{2})\pi}{a+1} \right\}. \tag{33}$$

Hence

$$\frac{1}{n} \log f_a \geqslant \frac{1}{4a^d} \sum_{m_1=0}^{a+b} \sum_{m_2=0}^{a+b} \dots \sum_{m_d=0}^{a+b} \log \left\{ 4 \sum_{i=1}^{d} \sin^2 \frac{(m_i + \frac{1}{2})\pi}{a+1} \right\}. \tag{34}$$

When $a \to \infty$, the left-hand side of (34) tends to λ_d and the right-hand tends to the corresponding multiple integral and we get (6). Equality holds in (6) in the particular case $d = 2$.

To compute the multiple integral (6) we proceed as follows.

$$\begin{aligned} K_d &= \frac{1}{4\pi^d} \int_0^\pi d\theta_1 \int_0^\pi d\theta_2 \dots \int_0^\pi d\theta_d \log \left\{ 4 \sum_{i=1}^{d} \sin^2 \theta_i \right\} \\ &= \frac{1}{4(2\pi)^d} \int_0^{2\pi} d\phi_1 \int_0^{2\pi} d\phi_2 \dots \int_0^{2\pi} d\phi_d \log \left\{ 2d - 2 \sum_{i=1}^{d} \cos \phi_i \right\} \quad (\phi_i = 2\theta_i) \\ &= \tfrac{1}{4} \log 2d - \frac{1}{4(2\pi)^d} \int_0^{2\pi} d\phi_1 \int_0^{2\pi} d\phi_2 \dots \int_0^{2\pi} d\phi_d \sum_{r=1}^{\infty} \frac{1}{r} \left(\frac{1}{d} \sum_{i=1}^{d} \cos \phi_i \right)^r \end{aligned} \tag{35}$$

on expanding the logarithm. Since

$$\frac{1}{2\pi} \int_0^{2\pi} \cos^m \theta \, d\theta = \begin{cases} 0 & m \text{ odd}, \\ 2^{-m} \binom{m}{\frac{1}{2}m} & m \text{ even} \end{cases} \tag{36}$$

we get, on expanding $(d^{-1} \Sigma \cos \phi_i)^r$ by the multinomial theorem and then integrating

$$K_d = \tfrac{1}{4} \log 2d - \frac{1}{4} \sum_{r=1}^{\infty} \frac{1}{2r} \frac{1}{d^{2r}} \Sigma_r \frac{(2r)!\,(2\rho_1)!\,(2\rho_2)! \dots (2\rho_d)!}{(2\rho_1)!\,(2\rho_2)! \dots (2\rho_d)!\, 2^{2r} (\rho_1!)^2 (\rho_2!)^2 \dots (\rho_d!)^2}, \tag{37}$$

where Σ_r denotes summation over all non-negative integers ρ_i such that

$$2\rho_1 + 2\rho_2 + \dots + 2\rho_d = 2r.$$

Hence

$$\lambda_d \geqslant K_d = \tfrac{1}{4} \log 2d - \frac{1}{8} \sum_{r=1}^{\infty} \frac{\gamma_r(d)}{r(2d)^{2r}} \binom{2r}{r}, \tag{38}$$

where $\gamma_r(d)$ is the sum of the squares of the coefficients in the multinomial expansion $(x_1 + x_2, + \dots + x_d)^r$.

I am indebted to Mr R. E. Thomas for evaluting K_3 from (38) on the Atlas computer at Chilton. This gives (5).

Postscript added in proof. I am indebted to Prof. J. F. C. Kingman for the remark that, if the van der Waerden conjecture is true, the inequality (6) can be sharpened considerably when $d \geqslant 4$. A matrix is said to be *doubly-stochastic* if its elements are non-

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negative and if each row and each column has unit sum: for instance, $\mathbf{V}^*/2d$ is doubly-stochastic, where $\mathbf{V}^*$ is the matrix in (12). The van der Waerden conjecture (which is very plausible, but has only been proved in a few special cases: see Marcus and Minc, *Amer. Math. Monthly* **72** (1965), 577–591) states that, if $\mathbf{A}$ is a doubly-stochastic matrix of order n, then $\operatorname{per}\mathbf{A} \geqslant n!/n^n$ with equality if and only if all elements of $\mathbf{A}$ are $1/n$. Assuming the conjecture, we get

$$\operatorname{per}\mathbf{V}^* = (2d)^n \operatorname{per}(\mathbf{V}^*/2d) \geqslant (2d)^n n!/n^n \geqslant (2d/e)^n;$$

and hence $\lambda_d \geqslant \frac{1}{2}\log(2d) - \frac{1}{2}$. This gives $\lambda_3 \geqslant 0{\cdot}396$, which is not as sharp as (5). However, for $d \geqslant 4$, it gives

$$K_d < \tfrac{1}{4}\log(2d) < \tfrac{1}{2}\log(2d) - \tfrac{1}{2} \leqslant \lambda_d$$

which is a great improvement on (6). Indeed, together with (1), we have

$$\tfrac{1}{2}\log d - 0{\cdot}153 \leqslant \lambda_d \leqslant \tfrac{1}{2}\log d,$$

which says a lot about λ_d for large d.

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