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1976 J. Phys. A: Math. Gen. 9 197

(http://iopscience.iop.org/0305-4470/9/2/002)

J. Phys. A: Math. Gen., Vol. 9, No. 2, 1976. Printed in Great Britain. © 1976

On an integral representation of the function Tr[exp($A - \lambda B$)]

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Received 20 May 1975, in final form 23 September 1975

Abstract. The conjecture that Tr[exp($A - \lambda B$)] can be written as a Laplace transform with a positive measure is proved for a certain class of matrices A and B. A few remarks are made about the undecided cases.

1. Introduction

In quantum statistical mechanics one deals with the partition function

$$Z = \mathrm{Tr}[\exp(-\beta H_0 - \beta\lambda V)]$$

where β and λ are real and the operators H_0 and V are Hermitian. In certain approximate procedures H_0 and V are taken to be finite dimensional. It has been observed by several authors that if Z can be written as a Laplace transform with a positive measure then one may use various inequalities known for the Padé approximants to derive bounds for Z (see e.g. Baker 1972a, b, Bessis 1974, Bessis *et al* 1975, Wheeler and Gordon 1970).

Motivated by this observation, Bessis (1975, private communication) (see also Bessis *et al* 1975) proposed the *conjecture* that, if A and B are finite Hermitian matrices, then

$$\mathrm{Tr}[\exp(A - \lambda B)] = \int_{b_<}^{b_>} \mathrm{e}^{-\lambda t}\, \mathrm{d}\mu(t) \qquad \mathrm{d}\mu \geqslant 0 \tag{1.1}$$

where all eigenvalues of B lie in the real interval $(b_<, b_>)$.

No counter examples are known and the conjecture may even be true for infinite dimensional matrices.

Since for any real numbers a and b and unit matrix I

$$\mathrm{Tr}\{\exp[(A + aI) - \lambda(B + bI)]\} = \exp(a - \lambda b)\, \mathrm{Tr}(A - \lambda B),$$

there is no loss of generality in assuming A and B to be positive definite. If A and B are finite positive definite Hermitian matrices the conjecture (1.1) is then equivalent to

$$\mathrm{Tr}[\exp(A - \lambda B)] = \int_0^{\infty} \mathrm{e}^{-\lambda t}\, \mathrm{d}\mu(t) \qquad \mathrm{d}\mu \geqslant 0. \tag{1.2}$$

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Further, since the trace is invariant under a unitary transformation of the matrices, we can take B to be diagonal.

The classes of matrices for which we can prove the conjecture are described in terms of the graph of matrix A, assumed positive definite and brought to the representation described in the previous paragraph.

A Hermitian matrix $A=[a_{ij}]$ of order N can be represented by a graph with N points. The point i is marked with the number a_{ii}. If $a_{ij}\neq 0$, the points i and j are joined by a line, which may be directed from i to j with the value of a_{ij} marked on it. Equivalently, one may direct the line from j to i and mark it with $a_{ji}=a_{ij}^*$. Thus there is a one-to-one correspondence between a matrix A and its marked graph.

Definition 1

A tree matrix is a matrix whose graph has no closed paths.

Definition 2

A matrix is said to have a real positive circuit if the product of the matrix elements taken along a closed path is real and positive. Similarly, a matrix is said to have a real negative circuit or a complex circuit according to whether the product of the matrix elements taken round a closed path is a real negative or a complex number.

We will show in the following that equations (1.1) and (1.2) are valid if the matrix A has only real non-negative circuits. In particular it will be the case when

(i) A is a tree matrix; there are no circuits, or all circuits are zero,
(ii) the off-diagonal part of A is separable; i.e. $a_{jk}=\alpha_j^*\alpha_k$ for $j\neq k$, and
(iii) the off-diagonal elements of A are all real and positive.

2. The proof using perturbation expansion

The conjecture is evidently true when A and B commute. In this section we first give (§ 2.1) the perturbation formula for the trace, and then prove (§ 2.2) the conjecture for the case when A has only one off-diagonal term. This is equivalent to proving the conjecture for all 2×2 matrices and introduces the procedure (§ 2.3) for proving the conjecture for cases mentioned in the introduction. In the last subsection (§ 2.4) we illustrate the difficulties of the general problem through the example of a 3×3 matrix.

2.1. *A perturbation series*

From the identity

$$\exp[u(X+Y)]=\exp(uX)+\int_0^u \exp[(u-u_1)X]\,Y\exp[u_1(X+Y)]\,du_1 \tag{2.1}$$

we deduce by recurrence and a change of variables the series expansion

$$e^{X+Y}=\sum_{n=1}^{\infty}\int_0^1\cdots\int_0^1 e^{Xv_1}Y\,e^{Xv_2}Y\ldots Y\,e^{Xv_n}\,\delta(v_1+\ldots+v_n-1)\prod_1^n dv_j. \tag{2.2}$$

Put

$$A-\lambda B = X + Y \tag{2.3}$$

where X and Y respectively are the diagonal and off-diagonal parts:

$$X=[x_i\delta_{ij}] \qquad x_i = a_{ii}-\lambda b_{ii} \equiv a_i - \lambda b_i \tag{2.4}$$

$$Y=[y_{ij}] \qquad y_{ij} = a_{ij}(1-\delta_{ij}) \tag{2.5}$$

and take matrix elements on both sides of equation (2.2):

$$\begin{aligned}[\exp(A-\lambda B)]_{ij} &= \sum_{n=1}^{\infty} \sum_{i_1,\ldots,i_n=1}^{N} \delta_{ii_1}\delta_{ji_n} a_{i_1i_2}a_{i_2i_3}\ldots a_{i_{n-1}i_n} \\ &\times \int_0^1 \ldots \int_0^1 \mathrm{d}v_1 \ldots \mathrm{d}v_n\, \delta(v_1+\ldots+v_n-1)\exp(x_{i_1}v_1+\ldots+x_{i_n}v_n).\end{aligned} \tag{2.6}$$

For every n, the nth order term on the right-hand side of equation (2.6) above can be represented by the path $(i, i_1, i_2, \ldots, i_{n-1}, j)$ traced on the graph of A.

2.2. The case when A has only one non-zero off-diagonal element

If $Y=0$, i.e. A and B commute, then only the term $n=1$ survives in the expansion (2.6), and we have

$$\mathrm{Tr}[\exp(A-\lambda B)] = \mathrm{Tr}(\mathrm{e}^X) = \sum_{i=1}^{N} \mathrm{e}^{x_i} = \int \mathrm{d}t\, \mathrm{e}^{-\lambda t}\mu_0(t), \tag{2.7}$$

$$\mu_0(t) = \sum_{i=1}^{N} \mathrm{e}^{a_i}\delta(t-b_i) \geqslant 0, \tag{2.8}$$

which has the form stipulated by equation (1.1). If $Y \neq 0$, then A and Y have the same graph. Let Y have only one non-zero matrix element, say, y_{12}. According to expansion (2.6) we have to calculate

$$\begin{aligned}&\int_0^1 \cdots \int_0^1 \mathrm{d}v_1 \ldots \mathrm{d}v_{2n+1}\, \delta(v_1+\ldots+v_{2n+1}-1)\exp\left(x_1 \sum_{i=0}^{n} v_{2i+1} + x_2 \sum_{i=1}^{n} v_{2i}\right) \\ &\quad = \int \ldots \int \exp[x_1 u + x_2(1-u)]\, \mathrm{d}u\, \mathrm{d}v_2 \ldots \mathrm{d}v_{2n}\end{aligned}$$

where the variables are restricted by the conditions

$$u \geqslant 0,\ v_2 \geqslant 0, \ldots, v_{2n} \geqslant 0 \qquad (v_3+v_5+\ldots+v_{2n-1}) \leqslant u \qquad (v_2+v_4+\ldots+v_{2n}) \leqslant 1-u.$$

This integral reduces to

$$\int_0^1 \mathrm{d}u\, \exp[x_1 u + x_2(1-u)] \frac{u^{n-1}(1-u)^n}{(n-1)!\,n!}, \tag{2.9}$$

which on symmetrization over x_1 and x_2 gives

$$\frac{1}{2}\int_0^1 \mathrm{d}u\, \exp[x_1 u + x_2(1-u)] \frac{u^{n-1}(1-u)^{n-1}}{(n-1)!\,n!}. \tag{2.10}$$

On replacing x_i by $a_i - \lambda b_i$ we have from (2.6) and (2.10)

$$\mathrm{Tr}[\exp(A-\lambda B)]$$
$$= \int e^{-\lambda t}\mu_0 \, dt + \sum_{n=1}^{\infty} \frac{|a_{12}|^{2n}}{n!(n-1)!} \int_0^1 du \exp[a_1 u + a_2(1-u) - \lambda b_1 u$$
$$- \lambda b_2(1-u)] u^{n-1}(1-u)^{n-1}. \tag{2.11}$$

The last relation is visibly of the form (1.1). In fact, if $b_1 \neq b_2$, one takes $b_1 u + b_2(1-u) = t$ as the new variable of integration and gets

$$\mathrm{Tr}[\exp(A-\lambda B)] = \int dt \, e^{-\lambda t}(\mu_0(t) + \mu_2(t)) \tag{2.12}$$

where $\mu_0(t)$ is given by equation (2.8) and

$$\mu_2(t) = F_{12}(t) G_{12}(t) \theta_{12}(t) \tag{2.13}$$

$$F_{ij}(t) = \exp\left[t\left(\frac{a_i - a_j}{b_i - b_j}\right) - \left(\frac{a_i b_j - a_j b_i}{b_i - b_j}\right)\right] \tag{2.14}$$

$$G_{ij}(t) = \sum_{n=1}^{\infty} \frac{|a_{ij}|^{2n}}{n!(n-1)!} \frac{(b_j - t)^{n-1}(t - b_i)^{n-1}}{(b_j - b_i)^{2n+1}} \tag{2.15}$$

$$\theta_{ij}(t) = \begin{cases} +1 & b_i < t < b_j \\ -1 & b_j < t < b_i \\ 0 & \text{otherwise.} \end{cases} \tag{2.16}$$

In case $b_1 = b_2$, the above substitution is singular, but then equation (2.12) is still valid with

$$\mu_2(t) = \delta(t - b_1) \sum_{n=1}^{\infty} \frac{|a_{12}|^{2n}}{n!(n-1)!} \int_0^1 \exp[a_1 u + a_2(1-u)] u^{n-1}(1-u)^{n-1} \, du. \tag{2.17}$$

$\mu_2(t) \geq 0$, whether it is given by equation (2.13) or by (2.17).

2.3. *The case of A having only real positive circuits*

Now let us consider the case when A (or Y) has many non-zero elements. The terms in the expansion (2.6) will be of the form

$$\mathrm{Tr}[\exp(A-\lambda B)]$$
$$= \sum_n \sum_{i_1, i_2, \ldots} |a_{i_1 i_2}|^{2j_1} \ldots (a_{i_r i_{r+1}} \ldots a_{i_s i_r})^p \ldots$$
$$\times \int_0^1 \ldots \int_0^1 \delta(\Sigma v_i - 1) \exp(x_{i_1} \Sigma v_{k_1} + x_{i_2} \Sigma v_{k_2} + \ldots) \, dv_1 \, dv_2 \ldots . \tag{2.18}$$

Some of the variables of integration will not occur explicitly in the exponential, others will stick together as sums. In any case, introducing

$$t=b_{i_1}\sum v_{k_1}+b_{i_2}\sum v_{k_2}+\dots \tag{2.19}$$

as one of the new variables of integration, we can transform the integral (2.18) to the form

$$\int\dots\int e^{-\lambda t}F(t, v_2, v_3, \dots, i_1, j_1, \dots)\,dt\,dv_2\,dv_3\dots \tag{2.20}$$

with $F\geqslant 0$. As t is a linear combination of b_i with coefficients which, though variable, always lie between 0 and 1, the range of variation of t will be confined to the spectrum of B. Therefore once the integrations over the remaining v_i are carried out, (2.20) will have the form

$$\int_{b_<}^{b_>} e^{-\lambda t}F(t, i_1, j_1, \dots)\,dt. \tag{2.21}$$

We have left out the trivial case when substitution (2.19) is singular.

If A has no circuits (i.e. is a tree matrix), or if it has only real positive circuits, then all the coefficients outside the integral in (2.18) are positive. Every term in the series expansion is of the form (1.1) and hence their sum is also of the same form.

This proves the conjecture for the three cases mentioned in the introduction.

2.4. *The case when A has real negative or complex circuits: example of a 3×3 matrix*

The situation is not clear when the circuits in A are not all real positive, for then there are terms corresponding to closed paths which may have either sign. For example, if $a_{12}a_{23}a_{31}\neq 0$ and negative or complex, there are terms of the general form

$$|a_{23}|^{2l}|a_{31}|^{2m}|a_{12}|^{2n}[(a_{12}a_{23}a_{31})^p+(a_{13}a_{32}a_{21})^p](J_1+J_2+J_3) \tag{2.22}$$

where

$$J_1=I_1\iiint_0^1 \delta(u+v+w-1)\exp(x_1u+x_2v+x_3w)$$

$$\times\frac{u^{m+n+p}}{(m+n+p)!}\,\frac{v^{n+l+p-1}}{(n+l+p-1)!}\,\frac{w^{l+m+p-1}}{(l+m+p-1)!}\,du\,dv\,dw \tag{2.23}$$

and $I_1\equiv I_1(l, m, n, p)$ is the number of distinct ways one can walk along the sides of the triangle (1, 2, 3) so as to start and finish at 1; the sides are traversed in the directions $2\to 3$, $3\to 1$ and $1\to 2$ $l+p$, $m+p$ and $n+p$ times, and in the opposite directions $3\to 2$, $1\to 3$ and $2\to 1$ l, m and n times respectively.

The quantities J_2 and J_3 are obtained from J_1 by circular permutations of (1, 2, 3).

We find (see appendix) that

$$I_1(l, m, n, p)=K(l, m, n, p)-K(l-1, m, n, p), \tag{2.24}$$

where

$$K(l, m, n, p)=\frac{(m+n+p)!(n+l+p)!(l+m+p)!}{(l+p)!(m+p)!(n+p)!l!m!n!}. \tag{2.25}$$

Collecting the above results we have

$$J_1+J_2+J_3=J_0\iiint_0^1 \delta(u+v+w-1)$$

$$\times (vw)^l(wu)^m(uv)^n(uvw)^{p-1}\exp(x_1u+x_2v+x_3w)\,du\,dv\,dw \tag{2.26}$$

$$=J_0\mathscr{D}\iiint_0^1 \delta(u+v+w-1)\exp(x_1u+x_2v+x_3w)\,du\,dv\,dw \tag{2.27}$$

$$=J_0\mathscr{D}D_{123}^{-1}\left(\int_{b_2}^{b_3} e^{-\lambda t}F_{23}\,dt+\int_{b_3}^{b_1} e^{-\lambda t}F_{31}\,dt+\int_{b_1}^{b_2} e^{-\lambda t}F_{12}\,dt\right) \tag{2.28}$$

with

$$J_0=J_0(l,m,n,p)=\frac{p^2+p(l+m+n)+mn+nl+lm}{(l+p)!(m+p)!(n+p)!\,l!\,m!\,n!} \tag{2.29}$$

$$\mathscr{D}=\mathscr{D}(l,m,n,p)=(\partial_2\partial_3)^l(\partial_3\partial_1)^m(\partial_1\partial_2)^n(\partial_1\partial_2\partial_3)^{p-1} \tag{2.30}$$

$$\partial_i=\partial/\partial a_i \qquad i=1,2,3 \tag{2.31}$$

$$D_{123}=a_1(b_2-b_3)+a_2(b_3-b_1)+a_3(b_1-b_2) \tag{2.32}$$

and F_{ij} is given by equation (2.14).

Summarizing the calculation of this section, for 3×3 matrices

$$A=\begin{bmatrix} a_1 & a_{12} & a_{13} \\ a_{21} & a_2 & a_{23} \\ a_{31} & a_{32} & a_3 \end{bmatrix}, \qquad B=\begin{bmatrix} b_1 & \cdot & \cdot \\ \cdot & b_2 & \cdot \\ \cdot & \cdot & b_3 \end{bmatrix} \tag{2.33}$$

and the complete perturbation series can be written as

$$\mathrm{Tr}[\exp(A-\lambda B)]=\int_{b_<}^{b_>} dt\, e^{-\lambda t}(\mu_0+\mu_2+\mu_3) \tag{2.34}$$

where

$$\mu_0=\sum_{i=1}^{3} e^{a_i}\delta(t-b_i)$$

$$\mu_2=\sum_{1\le i<j\le 3} F_{ij}(t)G_{ij}(t)\theta_{ij}(t) \tag{2.35}$$

$$\mu_3=\sum_{l,m,n,p=0}^{\infty} |a_{23}|^{2l}|a_{31}|^{2m}|a_{12}|^{2n}[(a_{12}a_{23}a_{31})^p+(a_{13}a_{32}a_{21})^p]J(l,m,n,p,t) \tag{2.36}$$

$$J(l,m,n,p,t)=J_0\mathscr{D}D_{123}^{-1}\sum_{1\le i<j\le 3} F_{ij}(t)\theta_{ij}(t) \tag{2.37}$$

with J_0, $\mathscr{D}$, D_{123}, F_{ij} and θ_{ij} given respectively by equations (2.29), (2.30), (2.32), (2.14) and (2.16).

Note that from equations (2.26)–(2.28) one has

$$J_1+J_2+J_3=\int_{b_<}^{b_>} \mathrm{d}t\, \mathrm{e}^{-\lambda t} J(l, m, n, p, t)$$

$$=J_0 \iiint_0^1 \delta(u+v+w-1) \exp(x_1 u+x_2 v+x_3 w)$$

$$\times u^{m+n+p-1} v^{n+l+p-1} w^{l+m+p-1}\, \mathrm{d}u\, \mathrm{d}v\, \mathrm{d}w, \tag{2.38}$$

and applying the arguments at the end of § 2.3 above one deduces that

$$J(l, m, n, p, t) \geqslant 0 \tag{2.39}$$

for any t and any non-negative integers l, m, n, p. The inequality (2.39) would be hard to deduce from equation (2.37).

Even with this we are not able to show that $\mu_0+\mu_2+\mu_3 \geqslant 0$.

3. Connection with the theorems of Bernstein and Bochner

Necessary and sufficient conditions under which a function $f(\lambda)$ admits a representation

$$f(\lambda)=\int_0^\infty \mathrm{e}^{-\lambda t}\, \mathrm{d}\mu(t) \qquad \mathrm{d}\mu \geqslant 0 \tag{3.1}$$

are well known. We were unable to apply the associated methods to find cases not covered in the previous sections. Indeed, one is led back to the same sort of manipulations and difficulties. It is of some interest to point out these connections.

Bernstein's theorem that the necessary and sufficient condition that $f(\lambda)$ be of the form (3.1) is that its successive derivatives alternate in sign, i.e.

$$(-1)^n \frac{\mathrm{d}^n}{\mathrm{d}\lambda^n} f(\lambda) \geqslant 0 \qquad n=0, 1, 2, \ldots \tag{3.2}$$

(see e.g. Widder 1971).

To apply the theorem we construct the successive derivatives as follows. Let $A-\lambda B=C$; then

$$D_n(\lambda, t)=(-1)^n \frac{\mathrm{d}^n}{\mathrm{d}\lambda^n} \mathrm{e}^{Ct}. \tag{3.3}$$

By considering the differential equation in t satisfied by $D_n(\lambda, t)$ we have the recursive relation

$$D_n(\lambda, t)=n \int_0^t \mathrm{d}t_1\, D_{n-1}(\lambda, t_1) B \exp[C(t-t_1)]$$

$$=n \int_0^t \mathrm{d}t_1 \exp[C(t-t_1)] B D_{n-1}(\lambda, t_1). \tag{3.4}$$

For the conjecture to hold we should be able to prove that

$$\mathrm{Tr}[D_n(\lambda, 1)] \geqslant 0 \tag{3.5}$$

for all n. While the D_n are Hermitian it was not possible to derive anything about (3.5) from the relations (3.4). On the other hand the iterated form

$$D_n(\lambda, t) = n! \int_0^t \mathrm{d}t_1 \int_0^{t_1} \mathrm{d}t_2 \ldots \int_0^{t_{n-1}} \mathrm{d}t_n\, B(t_n)B(t_{n-1}) \ldots B(t_2)B(t_1)\, \mathrm{e}^{Ct} \tag{3.6}$$

where $B(t) = \mathrm{e}^{Ct}B\mathrm{e}^{-Ct}$ leads us back to the perturbation formula of § 2. Indeed the graph of $C = A - \lambda B$ is the same as the graph of A, since B is assumed diagonal and one can prove the positivity of derivatives (3.5) for the same cases as before.

It is natural to consider the associated problem† utilizing Bochner's theorem. It has the added interest that one uses the spectral resolution of the operators in a way which suggests that the results may apply to infinite dimensional operators also.

If we consider the function

$$f(x) = \mathrm{Tr}[\exp(A + \mathrm{i}xB)] \tag{3.7}$$

for the real variable x and ask for the condition under which

$$f(x) = \int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}xw}\, \mathrm{d}F(w) \qquad \mathrm{d}F \geqslant 0 \tag{3.8}$$

we have Bochner's (1959) theorem.

Bochner's theorem.

Equation (3.8) holds if and only if

(i) $f(x)$ is continuous,

(ii) $|f(x)| \leqslant f(0)$ and

(iii) $f(x)$ is positive definite, i.e. for any positive integer N, and any set of complex numbers $\xi_1, \xi_2, \ldots, \xi_N$, and real numbers $x_1, x_2, \ldots, x_N$

$$S = \sum_{1 \leqslant \alpha, \beta \leqslant N} f(x_\alpha - x_\beta)\xi_\alpha \xi_\beta^* \geqslant 0. \tag{3.9}$$

Continuity is evident. One can verify also that

$$f(0) \geqslant |f(x)|$$

by using the product representation for the exponential

$$\exp(A + \mathrm{i}xB) = \lim_{n \to \infty} [\exp(A/n) \exp(\mathrm{i}xB/n)]^n$$

and Weyl's inequality (Weyl 1949, Thompson 1971, equation (42))

$$\mathrm{Tr}(MM^+)^s \geqslant |\mathrm{Tr}(M^{2s})|$$

for $s \to \infty$.

As may be expected the test for positive definiteness is not easy to apply. For purposes of orientation we observe that if

$$f(x) = \mathrm{Tr}[\mathrm{e}^A\, \mathrm{e}^{\mathrm{i}xB'}]$$

† For finite matrices, coefficients of λ^n in the power series expansion of $\mathrm{Tr}[\exp(A + \lambda B)]$ always exist, if these coefficients can be expressed as moments of a positive weight function on the full or half axis a representation of the form (3.8) or (1.2) will hold.

then the corresponding $S \geqslant 0$, as may be seen by using a representation in which B' is diagonal.

In the general case, using the product representation and B diagonal,

$$S = \lim_{n\to\infty} \sum_{j_1\ldots j_n} \mathscr{A}_{j_1 j_2 \ldots j_n} |\zeta_{j_1 j_2 \ldots j_n}|^2 \tag{3.10}$$

$$\mathscr{A}_{j_1 j_2 \ldots j_n} = [\exp(A/n)]_{j_1 j_2} [\exp(A/n)]_{j_2 j_3} \ldots [\exp(A/n)]_{j_n j_1} \tag{3.11}$$

$$\zeta_{j_1 j_2 \ldots j_n} = \sum_{\alpha} \xi_\alpha \exp[it_\alpha (b_{j_1} + b_{j_2} + \ldots + b_{j_n})/n]. \tag{3.12}$$

Since ζ is invariant under permutations of j and A is Hermitian the $\mathscr{A}$ always occur in complex conjugate pairs and S is real.

For the cases mentioned in § 1, it can be proved that the coefficients $\mathscr{A}_{j_1 j_2 \ldots j_n}$ are all positive so that $S \geqslant 0$; we omit the proofs.

4. Discussion

We have shown that the trace function admits a representation of form (1.2) for a non-trivial class of matrices. In attempting to extend this class the procedure of § 2 leads on the one hand to combinatorial problems of some complication and on the other to the problem of estimating certain integrals which appear to be generalizations of integrals which define hypergeometric functions.

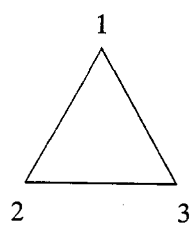
The approach through Bernstein's theorem using recursion relations (3.4) seems to require inequalities of an unusual type.

Acknowledgments

We are thankful to Professor K J LeCouteur for his interest in this problem.

Appendix

Let $I_1(l, m, n, p)$ be the number of ways of walking along the sides of the triangle (1, 2, 3), starting and ending the walk at corner 1, passing along sides $2\to 3$, $3\to 1$ and $1\to 2$ $l+p$, $m+p$ and $n+p$ times respectively, while in opposite directions $3\to 2$, $1\to 3$ and $2\to 1$ l, m and n times respectively.



From symmetry we have

$$I_1(l, m, n, p) = I_1(l, n, m, p) \tag{A.1}$$

$$I_1(l, m, n, -p) = I_1(l-p, m-p, n-p, p). \tag{A.2}$$

Also from elementary arguments one sees that

$$I_1(l, m, n, p) = \sum_{j=0}^{l} [I_1(j, m-1, n, p) + I_1(j, m, n-1, p) + I_1(j, m, n, p-1) + I_1(j-1, m-1, n-1, p+1)] + \delta_{m0}\delta_{n0}\delta_{p0}. \quad \text{(A.3)}$$

On replacing l by $l-1$ and subtracting we get

$$I_1(l, m, n, p) = I_1(l-1, m, n, p) + I_1(l, m-1, n, p) + I_1(l, m, n-1, p) + I_1(l, m, n, p-1) + I_1(l-1, m-1, n-1, p+1) + \delta_{m0}\delta_{n0}\delta_{p0}\delta_{l0}. \quad \text{(A.4)}$$

The boundary conditions are

$$I_1(l, m, n, p) = 0 \quad \text{(A.5)}$$

whenever one or more of the six integers l, m, n, $l+p$, $m+p$, $n+p$ is negative, or when $m=n=p=0$ and $l>0$.

As the value of $s = l+m+n+(l+p)+(m+p)+(n+p) = 2(l+m+n)+3p$ for each term on the right-hand side of (A.4) is strictly smaller than its value for the left-hand side, one can determine $I_1(l, m, n, p)$ step-by-step for all integers l, m, n and p starting from $l=m=n=p=0$. Any expression which satisfies the recurrence relation (A.4) and the boundary conditions (A.5) will therefore be unique. The following is such an expression as can be verified by direct substitution:

$$I_1(l, m, n, p) = K(l, m, n, p) - K(l-1, m, n, p) \quad \text{(A.6)}$$

where

$$K(l, m, n, p) = \frac{(m+n+p)!\,(n+l+p)!\,(l+m+p)!}{(l+p)!\,(m+p)!\,(n+p)!\,l!\,m!\,n!}. \quad \text{(A.7)}$$

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