Hence, we may replace (4.1) by

$$\left\{1 + \sum_{s=1}^{\infty} (-1)^s \frac{z^s}{(1-x^s)(1-y^s)}\right\} F^*(x,y,z) = 1. \tag{4.2}$$

Comparing (4.2) with (2.16) and (2.16)′, it follows at once that

$$f^*(n,p,k) = c(n,p,k), \tag{4.3}$$

where $f^*(n,p,k)$ is the limiting case ($m = \infty$) of $f(n,p,k)$; (4.3) is of course to be expected from the definitions.

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THE RECURRENCE RELATION $(r+1)f_{r+1} = xf_r' + (K-r+1)x^2 f_{r-1}$

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1. INTRODUCTION

In a recent note, in [3], Worster conjectured, on the basis of computer calculations, that for each positive integer k there exists an odd polynomial $Q_{2k-1}(x)$ of degree $2k-1$ such that, for every zero a of the Bessel function $J_0(x)$

$$\int_0^a Q_{2k-1}(x)[J_0(x)]^{2k}\,dx = [aJ_1(a)]^{2k}.$$

The conjecture was extended and proved in [1] the extended result being: for each positive k there exists an odd polynomial $Q(x)$, with nonnegative integer coefficients and of degree k or $k-1$ according to whether k is odd or even, such that for every zero a of $J_0(x)$

$$\int_0^a Q(x)[J_0(x)]^k\,dx = (k-1)![aJ_1(a)]^k. \tag{1.1}$$

If the factor $(k-1)!$ on the right-hand side is omitted, then the coefficients in $Q(x)$ are no longer integers. In addition, [1] also contained the following generalization due to Hammersley: if F_0, F_1, G_0, and G_1 are four functions of x such that

$$G_0\frac{dF_0}{dx} = -F_1, \qquad \frac{dF_1}{dx} = G_1F_0,$$

and $F_0(a) = G_0(0) = 0$, so that $F_1(0) = 0$,

then there exists $Q(x)$ depending only on G_0, G_1, and K with the property

(1.2) $$(k - 1)![F_1(a)]^k = \int_0^a Q(x)[F_0(x)]^k dx.$$

As is observed in [1], Worster's extended conjecture corresponds to the case $G_0(x) = G_1(x) = x$.

Subsequently there has been some interest (see [2]) in the determination of the coefficients occurring in the Worster polynomial $Q(x)$. In this paper we show that by considering a certain recurrence relation, namely that given in the title, the coefficients can be expressed as multiple sums. Also, we show how to determine these multiple sums analytically and numerically. To obtain the recurrence relation, which is central to the work, we first consider an alternative proof to that given in [1] of Hammersley's generalization of Worster's conjecture.

SECTION 2

We begin by defining the function $\phi(x)$ by

$$\phi(x) = \sum_{r=0}^{k} f_r(x) F_0^r(x) F_1^{k-r}(x),$$

where $f_0(x), f_1(x), \ldots, f_k(x)$ is some sequence of functions which, for the moment we leave unspecified. Differentiating the expression for $\phi(x)$, and omitting the argument x occurring in the various functions, we have

$$\phi' = \sum_{r=0}^{k} \left\{ f_r' F_0^r F_1^{k-r} + f_r (r F_0^{r-1} F_0' F_1^{k-r} + (k - r) F_0^r F_1^{k-r-1} F_1') \right\}.$$

Since $G_0 F_0' = -F_1$ and $F_1' = G_1 F_0$, we obtain

$$\phi' = \sum_{r=0}^{k} \left\{ f_r' F_0^r F_1^{k-r} - \frac{r f_r}{G_0} F_0^{r-1} F_1^{k-r-1} + (k - r) f_r G_1 F_0^{r+1} F_1^{k-r+1} \right\}.$$

This can be put in the alternative and more convenient form

$$\phi' = \left\{ f_0' - \frac{f_1}{G_0} \right\} F_1^k + \sum_{r=1}^{k-1} \left[f_r' - \frac{(r + 1)}{G_0} f_{r+1} + (k - r + 1) f_{r-1} G_1 \right] F_0^r F_1^{k-r} + (f_k' + f_{k-1} G_1) F_0^k.$$

We put $f_0 = (k - 1)!$ and choose the functions $f_1, f_2, \ldots, f_k$ so that the coefficients of $F_0^r F_1^{k-r}$, $r = 0, 1, 2, \ldots, k - 1$ vanish. It immediately follows that $f_1 = 0$, while

(2.1) $$(r + 1) f_{r+1} = G_0 \left\{ f_r' + (k - r + 1) f_{r-1} G_1 \right\}, \quad r = 1, 2, \ldots, k - 1.$$

The sequence of functions $f_0, f_1, \ldots, f_k$ is now completely defined, and it clearly depends only on k, G_0, and G_1. For $r \geq 2$, $f_r(0) = 0$ since $G_0(0) = 0$.

The expression for ϕ' reduces to

(2.2) $$\phi' = (f_k' + f_{k-1} G_1) F_0^k.$$

Integrating (2.2) with respect to x between 0 and a, we obtain, reinserting arguments where appropriate,

$$\left[\sum_{r=0}^{k} f_r(x)F_0^r(x)F_1^{k-r}(x)\right]_0^a = \int_0^a (f_k' + f_{k-1}G_1)F_0^k dx.$$

Using the properties of the various functions on the left-hand side of this equation, we deduce

$$(k-1)!F_1^k(a) = \int_0^a (f_k' + f_{k-1}G_1)F_0^k dx.$$

Hence, the generalization stated in (2.2) follows immediately if we take

$$Q(x) = f_k' + f_{k-1}G_1.$$

If we define f_{k+1} by putting $r = k$ in (2.1), then

$$Q(x) = \frac{(k+1)}{G_0} f_{k+1}.$$

Omitting the factor $(k-1)!$ occurring in (1.1) we see that the determination of $Q(x)$ for the Worster problem is achieved by solving

$$\begin{aligned} &f_0 = 1, \quad f_1 = 0 \\ (2.3) \qquad &(r+1)f_{r+1} = xf_r' + (k - r + 1)x^2 f_{r-1}, \; r = 1, 2, \ldots, k \\ &xQ(x) = (k+1)f_{k+1} \end{aligned}$$

The following are readily deduced:

$$\begin{aligned} &f_2 = \frac{kx^2}{2!}, \; f_3 = \frac{2kx^2}{3!}, \; f_4 = \frac{2^2kx^2}{4!} + 3k(k-2)\frac{x^4}{4!} \\ (2.4) \qquad &f_5 = \frac{2^3kx^2}{5!} + \left\{3\cdot 4k(k-2) + 2\cdot 4k(k-3)\right\}\frac{x^4}{5!} \\ &f_6 = \frac{2^4kx^2}{6!} + \left\{3\cdot 4^2k(k-2) + 2\cdot 4^2k(k-3) + 2^2 5k(k-4)\right\}\frac{x^4}{6!} \\ &\qquad + 3\cdot 5k(k-2)(k-4)\frac{x^6}{6!} \end{aligned}$$

Thus, we can find the first four of the polynomials $Q(x)$. These correspond to $k = 2, 3, 4$, and 5, respectively. We now proceed to establish a number of results concerning the functions f_r. From these, we deduce expressions for the coefficients of the powers of x in $Q(x)$.

SECTION 3

It is first convenient to prove the following results for multiple sums

$$(3.1) \qquad \sum_{q=3}^{n-1}\sum_{p=q+2}^{n+1} a_{qp} = \sum_{q=3}^{n-2}\sum_{p=q+2}^{n} a_{qp} + \sum_{q=3}^{n-1} a_{q,n+1}$$

and

$$(3.2) \qquad \sum_{q=3}^{n-3}\sum_{p=q+2}^{n-1}\sum_{\ell=p+2}^{n+1} a_{qp\ell} = \sum_{q=3}^{n-4}\sum_{p=q+2}^{n-2}\sum_{\ell=p+2}^{n} a_{qp\ell} + \sum_{q=3}^{n-3}\sum_{p=q+2}^{n-1} a_{qp,n+1}.$$

We have

$$\sum_{q=3}^{n-2}\sum_{p=q+2}^{n} a_{qp} = \sum_{q=3}^{n-2}\left\{\sum_{p=q+2}^{n+1} a_{qp} - a_{q,n+1}\right\} = \left\{\sum_{q=3}^{n-1} - \sum_{q=n-1}^{n-1}\right\}\left\{\sum_{p=q+2}^{n+1} a_{qp}\right\} - \sum_{q=3}^{n-2} a_{q,n+1}.$$

When $q = n-1$, p can only take the value $n+1$, so that the above expression reduces to

$$\sum_{q=3}^{n-1}\sum_{p=q+2}^{n+1} a_{qp} - a_{n-1,n+1} - \sum_{q=3}^{n-2} a_{q,n+1} = \sum_{q=3}^{n-1}\sum_{p=q+2}^{n+1} a_{qp} - \sum_{q=3}^{n-1} a_{q,n+1}.$$

Thus the result given in (3.1) now follows. To prove (3.2) we proceed similarly.

$$\sum_{q=3}^{n-4}\sum_{p=q+2}^{n-2}\sum_{\ell=p+2}^{n} a_{qp\ell} = \sum_{q=3}^{n-4}\sum_{p=q+2}^{n-2}\left\{\sum_{\ell=p+2}^{n+1} - \sum_{\ell=n+1}^{n+1}\right\} a_{qp\ell}$$

$$= \sum_{q=3}^{n-4}\left\{\sum_{p=q+2}^{n-1} - \sum_{p=n-1}^{n-1}\right\}\sum_{\ell=p+2}^{n+1} a_{qp\ell} - \sum_{q=3}^{n-4}\sum_{p=q+2}^{n-2} a_{qp,n+1}$$

$$= \sum_{q=3}^{n-4}\sum_{p=q+2}^{n-1}\sum_{\ell=p+2}^{n+1} a_{qp\ell} - \sum_{q=3}^{n-4} a_{q,n-1,n+1} - \sum_{q=3}^{n-4}\sum_{p=q+2}^{n-2} a_{qp,n+1}$$

since ℓ can only take the value $n+1$ when $p = n-1$. Continuing, we have

$$\sum_{q=3}^{n-4}\sum_{p=q+2}^{n-2}\sum_{\ell=p+2}^{n} a_{qp\ell} = \sum_{q=3}^{n-3}\sum_{p=q+2}^{n-1}\sum_{\ell=p+2}^{n+1} a_{qp\ell} - a_{n-3,n-1,n+1} - \sum_{q=3}^{n-4} a_{q,n-1,n+1} - \sum_{q=3}^{n-4}\sum_{p=q+2}^{n-2} a_{qp,n+1}$$

(3.3)

$$= \sum_{q=3}^{n-3}\sum_{p=q+2}^{n-1}\sum_{\ell=p+2}^{n+1} a_{qp\ell} - \sum_{q=3}^{n-3} a_{q,n-1,n+1} - \sum_{q=3}^{n-4}\sum_{p=q+2}^{n-2} a_{qp,n+1}.$$

Using (3.1) with $a_{qp,n+1}$ instead of a_{qp} and n replaced by $n-2$ now leads us directly to (3.2). The results given in (3.1) and (3.2) can be extended to quadruple and higher-tuple sums. Thus, for quadruple sums the analogous result to (3.3) is

$$\sum_{q=3}^{n-6}\sum_{p=q+2}^{n-4}\sum_{\ell=p+2}^{n-2}\sum_{j=\ell+2}^{n} a_{qp\ell j}$$

$$= \sum_{q=3}^{n-5}\sum_{p=q+2}^{n-3}\sum_{\ell=p+2}^{n-1}\sum_{j=\ell+2}^{n+1} a_{qp\ell j} - a_{n-5,n-3,n-1,n+1} - \sum_{q=3}^{n-6} a_{q,n-3,n-1,n+1} - \sum_{q=3}^{n-4}\sum_{p=q+2}^{n-6} a_{qp,n-1,n+1} - \sum_{q=3}^{n-6}\sum_{p=q+2}^{n-4}\sum_{\ell=p+2}^{n-2} a_{qp\ell,n+1}.$$

If we now apply (3.1) and (3.2) to this equation, we obtain the result for the quadruple sum. The general result for p-tuple sums can be written as follows:

(3.4)

$$\sum_{q_1=3}^{n-2p+3}\sum_{q_2=q_1+2}^{n-2p+5}\cdots\sum_{q_i=q_{i-1}+2}^{n-2p+2i+1}\cdots\sum_{q_p=q_{p-1}+2}^{n+1} a_{q_1q_2\cdots q_p} = \sum_{q_1=3}^{n-2p+2}\sum_{q_2=q_1+2}^{n-2p+4}\cdots\sum_{q_i=q_{i-1}+2}^{n-2p+2i}\cdots\sum_{q_p=q_{p-1}+2}^{n} a_{q_1q_2\cdots q_p} + \sum_{q_1=3}^{n-2p+3}\sum_{q_2=q_1+2}^{n-2p+5}\cdots\sum_{q_{p-1}=q_{p-2}+2}^{n-1} a_{q_1q_2,q_{p-1},n+1}.$$

The first of our results concerning the sequence of functions f_r is

(i) f_{2r}, f_{2r+1}, where $r \geq 1$, are even polynomials of degree $2r$, the least power in each being that of x^2. This can be readily established using the recurrence relation in (2.3), the expressions in (2.4), and induction. Next, we prove:

(ii) the coefficient of x^2 in f_{r+1} is $\dfrac{2^{r-1}k}{(r+1)!}$, $r = 1, 2, 3, \ldots$.

From the recurrence relation (2.3), we have that

$$f_{r+2} = \frac{x}{r+2}f'_{r+1} + \frac{x^2(k-r)}{r+2}f_r$$

Hence we see, with the help of (i), that the term in x^2 in f_{r+2} will arise from differentiating the term in x^2 in f_{r+1} and multiplying by

$$\frac{x}{r+2}.$$

Assuming the result stated in (ii) is true for a specific r, then we have that the coefficient of x^2 in f_{r+2} is

$$\frac{2^r k}{(r+2)!}.$$

Thus, induction with the aid of (2.4) completes the proof.

(iii) The coefficient of x^4 in f_{r+1} is

$$\frac{k}{(r+1)!}\sum_{q=3}^{r} q(k-q+1)4^{r-q}2^{q-3},\ r \geq 3.$$

From the recurrence relation, we observe that the term in x^4 in f_{r+2} arises from the term in x^2 in f_r and the differentiation of the term in x^4 in f_{r+1}. Assuming that (iii) is true for fixed r, then we have with the aid of (ii) that the coefficient of x^4 in f_{r+2} is

$$\frac{(k-r)2^{r-2}k}{(r+2)r!} + \frac{4k}{(r+2)!}\sum_{q=3}^{r} q(k-q+1)4^{r-q}2^{q-3}$$

which reduces to

$$\frac{k}{(r+2)!}\sum_{q=3}^{r+1} q(k-q+1)4^{r+1-q}2^{q-3}.$$

Noting the expression for f_4 in (2.4) we see that induction completes our proof.

(iv) The coefficient of x^6 in f_{r+1} for $r \geq 5$ is

$$\frac{k}{(r+1)!}\sum_{q=3}^{r-2}\ \sum_{p=q+2}^{r} q(k-q+1)p(k-p+1)6^{r-p}4^{p-q-2}2^{q-3}.$$

The recurrence formula shows that to obtain the term in x^6 in f_{r+2} we must consider the term in x^4 in f_r and the result of differentiating the term in x^6 in f_{r+1}. If (iv) holds for a definite r then the coefficient of x^6 in f_{r+2} is seen, with the help of (iii), to be

$$\begin{aligned}&\frac{k-r}{r+2}\,\frac{k}{r!}\sum_{q=3}^{r-1} q(k-q+1)4^{r-1-q}2^{q-3}\\ &+\frac{6k}{(r+2)!}\sum_{q=3}^{r-2}\ \sum_{p=q+2}^{r} q(k-q+1)p(k-p+1)6^{r-p}4^{p-q-2}2^{q-3}\\ &=\frac{k}{(r+2)!}\sum_{q=3}^{r-1}(k-r)(r+1)q(k-q+1)4^{r-1-q}2^{q-3}\\ &+\sum_{q=3}^{r-2}\ \sum_{p=q+2}^{r} q(k-q+1)p(k-p+1)6^{r+1-p}4^{p-q-2}2^{q-3}.\end{aligned}$$

If we take

$$a_{qp} = q(k-q+1)p(k-p+1)6^{r+1-p}4^{p-q-2}2^{q-3},$$

we find

$$a_{q,r+1} = q(k-r)(r+1)q(k-q+1)4^{r-1-q}2^{q-3},$$

so that applying (3.1) with r instead of n we have the required coefficient of x^6 in f_{r+2}:

$$\frac{k}{(r+2)!}\sum_{q=3}^{r-1}\ \sum_{p=q+2}^{r+1} q(k-q+1)p(k-p+1)6^{r+1-p}4^{p-q-2}2^{q-3}.$$

Induction now completes our proof.

(v) The coefficient of x^{2r} in f_{2r}, $r \geq 3$, is

$$\frac{\left(\frac{k}{2}\right)!}{r!\left(\frac{k}{2}-r\right)!}$$

When k is odd, we take $\left(\frac{k}{2}\right)!$ and $\left(\frac{k}{2}-r\right)!$ to be generalized factorial functions. Use of the recurrence relation (2.3) yields

$$f_{2r+2} = \frac{x}{2r+2}f_{2r+1}' + x^2\,\frac{(k-2r)}{2r+2}f_{2r}.$$

Noting (i), we see that it is the term

$$\frac{x^2(k-2r)}{2r+2}f_{2r}$$

which gives rise to the power x^{2r+2} in f_{2r+2}. Thus if (v) is correct for fixed r, then the coefficient of x^{2r+2} in f_{2r+2} is

$$\frac{(k-2r)\left(\frac{k}{2}\right)!}{(2r+2)r!\left(\frac{k}{2}-r\right)!} = \frac{\left(\frac{k}{2}\right)!}{(r+1)!\left(\frac{k}{2}-r-1\right)!}$$

Once more induction, with the help of the expression for f_6 in (2.4), completes our proof.

(vi) The coefficient of x^{2t} in f_{r+1}, $3 \le t \le \left[\frac{r+1}{2}\right]$, $r \ge 5$, ..., is given by $S(r,t)$ where

$$S(r,t) = \frac{k}{(r+1)!} \sum_{q_1=3}^{r-2t+4} \sum_{q_2=q_1+2}^{r-2t+6} \cdots \sum_{q_i=q_{i-1}+2}^{r-2t+2i+2} \cdots \sum_{q_{t-1}=q_{t-2}+2}^{r} a_{q_1 q_2 \cdots q_{t-1}}(r,t)$$

and

$$a_{q_1 q_2 \cdots q_{t-1}}(r,t) = (2t)^{r-q_{t-1}} 2^{q_1-3} \prod_{j=1}^{t-1} q_j(k - q_j + 1) \prod_{j=2}^{t-1} (2j)^{q_j - q_{j-1} - 2}.$$

From the given expression, it is evident that $S(r,t)$ is a $(t-1)$-tuple sum. It is readily verified that (vi) reduces to (iv) when $t = 3$. Further, some elementary manipulation shows that:

$$S(2r-1,r) = \frac{\left(\frac{k}{2}\right)!}{r!\left(\frac{k}{2} - r\right)!}$$

so that (vi) also agrees with the result in (v). It is perhaps worth noting that the q_i in this latter case each take just one value, viz. $q_i = 1 + 2i$ $(i = 1, 2, \ldots, r-1)$. To prove (vi) we first show that if for fixed r and t the coefficients of x^{2t} in f_r and x^{2t-2} in f_{r-1} are given, respectively, by $S(r,t)$ and $S(r-1,t-1)$ then $S(r+1,t)$ is the coefficient of x^{2t} in f_{r+2}. Using the recurrence relation (2.3) in the form

$$f_{r+2} = \frac{x}{r+2} f'_{r+1} + \frac{k - r + 1}{r+2} x^2 f_r$$

we have that the coefficient of x^{2t} in f_{r+2} is

$$\frac{2t}{r+2} S(r,t) + \frac{k-r+1}{r+2} S(r-1,t-1)$$

which is equal to

$$\frac{k}{(r+2)!} \left\{ \sum_{q_1=3}^{r-2t+4} \cdots \sum_{q_{t-1}=q_{t-2}+2}^{r} a_{q_1 q_2 \cdots q_{t-1}}(r+1,t) + \right. \tag{3.5}$$
$$\left. \sum_{q_1=3}^{r-2t+5} \cdots \sum_{q_{t-2}=q_{t-3}+2}^{r-1} \{a_{q_1 q_2 \cdots q_{t-2}}(r-1,t-1)\}(k-1+1)(r+1) \right\}$$

Now

$$\begin{aligned} &a_{q_1 q_2 \cdots q_{t-2}, r+1}(r+1,t) \\ &= 2^{q_1-3}(r+1)(k-r+1) \prod_{j=1}^{t-2} q_j(k - q_j + 1) \\ &\qquad \times \prod_{j=2}^{t-2} (2j)^{q_j - q_{j-1} - 2} (2t-2)^{r-1-q_{t-2}} \\ &= (k-r+1)(r+1) a_{q_1, q_2, \ldots, q_{t-2}}(r-1,t-1). \end{aligned}$$

Hence, using (3.4) with n replaced by r and p by $t-1$ we can see that (3.5) reduces to $S(r+1,t)$. As already observed, the formula shown in (vi) correctly gives the coefficient of x^6 in $f_6, f_7, f_8, \ldots$, and also the coefficients of x^8 in f_8, x^{10} in f_{10}, x^{12} in f_{12}, etc. Hence by the result just proved with $2t = r = 8$ (vi) correctly gives the coefficient of x^8 in f_9. Applying the result again with $2t = r - 1 = 8$, we see that formula (vi) correctly gives the coefficient of x^8 in f_{10}. Thus, continuing the process, we prove that formula (vi) is also correct for the coefficient of x^8 in $f_{11}, f_{12}, \ldots$. The process is now repeated, starting with $2t = r = 10$. By this means, we successively establish the formula for the coefficients of x^8, x^{10}, x^{12}, etc.

From (2.3) we have $xQ(x) = (k+1)f_{k+1}$, so that it is now possible to deduce a number of results concerning $Q(x)$. These are:

the coefficient of x is $\dfrac{2^{k-1}}{(k-1)!}$,

that of x^3 is $\dfrac{1}{(k-1)!}\sum_{q=3}^{k} q(k-q+1)4^{k-q}2^{q-3}$, and

that of x^{2t-1} $(t \geq 3)$ is the $(t-1)$-tuple sum

$$\frac{1}{(k-1)!}\sum_{q_1=3}^{k-2t+4}\ \sum_{q_2=q_1+2}^{k-2t+6}\cdots\sum_{q_{t-1}=q_{t-2}+2}^{k} a_{q_1q_2\cdots q_{t-1}}(k,t)$$

where

$$a_{q_1q_2\cdots q_{t-1}}(k,t) = (2t)^{k-q_{t-1}}\,2^{q_1-3}\prod_{j=1}^{t-1} q_j(k-q_j+1) \times \prod_{j=2}^{t-1}(2j)^{q_j-q_{j-1}-2}.$$

In the next section we show how the multiple sums can be determined and find them in certain cases.

SECTION 4

Referring to the end of the last section we see that the coefficient of x^3 in $Q(x)$ can be written as

$$\frac{2^{k-3}}{(k-1)!}S(k)$$

where

(4.1) $$S(k) = \sum_{q=3}^{k} q(k-q+1)2^{k-q}.$$

We now put

(4.2) $$S(k) = kS_1(k) - S_2(k)$$

where

(4.3) $$S_1(k) = \sum_{q=3}^{k} q2^{k-q}$$

and

(4.4) $$S_2(k) = \sum_{q=3}^{k} q(q-1)2^{k-q}.$$

These series have the sums

(4.5) $$S_1(k) = 2^k - k - 2$$

and

(4.6) $$S_2(k) = 72^{k-1} - k^2 - 3k - 4.$$

Hence

$$S(k) = (2k - 7)2^{k-1} + k + 4,$$

giving the coefficient of x^3 as

$$\frac{2^{k-3}}{(k-1)!}\{2^{k-1}(2k-7) + k + 4\}.$$

It is perhaps worth noting that this expression vanishes for $k = 1$ and 2.

Again referring to the end of Section 3, we see that the coefficient of x^5 in $Q(x)$ can be written as

$$\frac{2^{k-5}}{(k-1)!}T(k),$$

where

$$T(k) = \sum_{q=3}^{k-2}\sum_{p=q+2}^{k}\{kq - q(q-1)\}\{kp - p(p-1)\}3^{k-p}2^{p-q-2}.$$

Putting

(4.7) $$T(k) = k^2T_1(k) - kT_2(k) + T_3(k),$$

then

(4.8) $$T_1(k) = \sum_{q=3}^{k-2}\sum_{p=q+2}^{k} pq3^{k-p}2^{p-q-2}$$

(4.9) $$T_2(k) = \sum_{q=3}^{k-2}\sum_{p=q+2}^{k}\{pq(q-1) + qp(p-1)\}3^{k-p}2^{p-q-2},$$

and

(4.10) $$T_3(k) = \sum_{q=3}^{k-2}\sum_{p=q+2}^{k} q(q-1)p(p-1)3^{k-p}2^{p-q-2}.$$

With the help of (3.1), (4.3), (4.4), and (4.8) to (4.10), we deduce

(4.11) $$\begin{aligned} T_1(k) &= 3T_1(k-1) + kS_1(k-2) \\ T_2(k) &= 3T_2(k-1) + k(k-1)S_1(k-2) + kS_2(k-2) \\ T_3(k) &= 3T_3(k-1) + k(k-1)S_2(k-2). \end{aligned}$$

Since $T_1(5) = 15$, $T_2(5) = 90$, and $T_3(5) = 120$, these recurrence relations enable us, with the help of (4.5) and (4.6), to find $T_1(k)$, $T_2(k)$, and $T_3(k)$ numerically, and hence, from (4.7), we can determine $T(k)$. We can also use the recurrence relations to find analytical expressions for the $T_i(k)$, $i = 1, 2, 3$. The method is the same in each instance. Therefore, we illustrate it by considering $T_1(k)$, then stating corresponding results for $T_2(k)$ and $T_3(k)$. The method depends on recognizing that the recurrence relation (4.11) and the condition $T_1(5) = 15$ can be satisfied by taking $T_1(k)$ in the form

(4.12) $$T_1(k) = f_3(k)3^k + f_2(k)2^k + f_1(k),$$

where $f_1(k)$, $f_2(k)$, and $f_3(k)$ are polynomials in k. It is perhaps worth emphasizing that once we have a solution for $T_1(k)$ it will be the solution. Inspection suggests we write

$$T_1(k) = a_0 3^k + (b_0 + b_1 k)2^k + c_0 + c_1 k + c_2 k^2. \tag{4.13}$$

From (4.11) and (4.5), we have

$$\begin{aligned} a_0 3^k &+ (b_0 + b_1 k)2^k + c_0 + c_1 k + c_2 k^2 \\ &= a_0 3^k + \frac{3}{2}(b_0 + b_1(k - 1))2^k + 3(c_0 + c_1(k - 1) \\ &\qquad + c_2(k - 1))^2 + k(2^{k-2} - k). \end{aligned}$$

Comparing coefficients, we obtain

$$b_1 = -\frac{1}{2},\ b_0 = -\frac{3}{2},\ c_2 = \frac{1}{2},\ c_1 = \frac{3}{2},\ \text{and } c_0 = \frac{3}{2}$$

while a_0 is indeterminate. To obtain a_0 we can proceed in two ways. First, we calculate a_0 from (4.13) by putting $k = 5$ and noting that $T_1(5) = 15$. This gives $a_0 = 1/2$. Second, we observe that we can regard $T_1(k)$ as being defined for all k by (4.5), (4.11), and $T_1(5) = 15$; thus, determine $T_1(0)$ and so obtain a_0 by putting $k = 0$ in (4.13). This is a somewhat easier procedure to carry out computationally than the first. It is readily found that $T_1(4) = T_1(3) = 0$, $T_1(2) = T_1(1) = 1$, and $T_1(0) = 1/2$, again giving us $a_0 = 1/2$. So,

$$T_1(k) = \frac{1}{2}3^k - (k + 3)2^{k-1} + \frac{1}{2}(k^2 + 3k + 3). \tag{4.14}$$

Likewise, we find $T_2(4) = T_2(3) = T_3(4) = T_3(3) = 0$, $T_2(2) = 3$, $T_2(1) = 2$, $T_2(0) = 3/4$, $T_3(2) = 2$, $T_3(1) = 1$, and $T_3(0) = 1/3$. Assuming appropriate forms for $T_2(k)$ and $T_3(k)$, we obtain

$$T_2(k) = \frac{21}{4}3^k - (2k^2 + 17k + 45)2^{k-2} + k^3 + \frac{7k^2}{2} + 7k + \frac{27}{4} \tag{4.15}$$

and

$$\begin{aligned} T_3(k) = \frac{139}{4}3^{k-1} - 7(k^2 + 5k + 12)2^{k-2} + \frac{k^4}{2} + 2k^3 \\ + 6k^2 + 11k + \frac{39}{4} \end{aligned} \tag{4.16}$$

so that the coefficient of x^5 is

$$\begin{aligned} \frac{2^{k-7}}{(k - 1)!}\{3^{k-1}(6k^2 - 63k + 139) + 2^{k+1}(2k - 7)(k + 6) \\ + 2k^2 + 17k + 39\}. \end{aligned}$$

We note that this last expression vanishes for $k = 1, 2, 3$, and 4.

We now proceed to find the coefficient of x^7 in $Q(x)$. Since the procedure is similar to that for finding the coefficient of x^5, we merely state the essential results. Suffix notation employed in the expression for the coefficient of x^{2t-1} $(t \geq 3)$ is not used here; it is sufficient to write the coefficient of x^7 as

$$\frac{2^{k-7}}{(k - 1)!}R(k)$$

where

$$R(k) = \sum_{q=3}^{k-4} \sum_{p=q+2}^{k-2} \sum_{r=p+2}^{k} \{kq - q(q-1)\}\{kp - p(p-1)\}\{kr - r(r-1)\}4^{k-r}3^{r-p-2}2^{p-q-2}$$

$$= k^3 R_1(k) - k^2 R_2(k) + kR_3(k) - R_4(k).$$

Now

$$R_1(k) = 4R_1(k-1) + kT_1(k-2)$$
$$R_2(k) = 4R_2(k-1) + k(k-1)T_1(k-2) + kT_2(k-2)$$
$$R_3(k) = 4R_3(k-1) + k(k-1)T_2(k-2) + KT_3(k-2)$$
$$R_4(k) = 4R_4(k-1) + k(k-1)T_3(k-2).$$

We deduce, with the help of the results for $T_i(k)$,

$$R_1(0) = -\frac{1}{6},\ R_2(0) = -\frac{1}{2},\ R_3(0) = -\frac{41}{72},\ R_4(0) = -\frac{11}{48}.$$

Again, making appropriate choice of forms, we obtain

$$R_1(k) = \frac{4^k}{6} - \frac{3^{k-1}}{2}(k+4) + 2^{k-3}(k^2 + 5k + 8) - \frac{k^3}{6} - \frac{k^2}{2} - \frac{5k}{6} - \frac{2}{3}$$

$$R_2(k) = \frac{7}{2}4^k - \frac{3^{k-1}}{4}\{2k^2 + 35k + 132\} + 2^{k-4}\{4k^3 + 33k^2 + 125k + 192\} - \frac{k^4}{2} - \frac{3k^3}{2} - 4k^2 - \frac{27k}{4} - 5$$

$$R_3(k) = \frac{1553}{72}4^k - 3^k\left\{\frac{7k^2}{9} + \frac{145k}{9} + \frac{517}{9}\right\} + 2^{k-4}\{2k^4 + 30k^3 + 173k^2 + 551k + 812\} - \frac{k^5}{2} - \frac{3k^4}{2} - \frac{35k^3}{6} - \frac{57k^2}{4} - 21k - \frac{139}{9}$$

$$R_4(k) = \frac{16277}{432}4^k - \frac{139}{4}3^{k-2}(k^2 + 7k + 24) + 72^{k-4}(k^4 + 8k^3 + 41k^2 + 118k + 168) - \frac{k^6}{6} - \frac{k^5}{2} - \frac{8k^4}{3} - \frac{25k^3}{3} - \frac{73k^2}{4} - \frac{947k}{36} - \frac{506}{27}$$

so that the coefficient of x^7 is

$$\frac{2^{k-9}}{3(k-1)!}\left[4^k\left\{2k^3 - 42k^2 + \frac{1553k}{6} - \frac{16277}{36}\right\} + 3^k(k+8)(6k^2 - 63k + 139 + 32^{k-1}(2k-7)(2k^2 + 25k + 84) + 2k^3 + 27k^2 + \frac{391k}{3} + \frac{2024}{9}\right]$$

This expression vanishes when $k = 1, 2, 3, 4, 5$, and 6. We could now proceed, in a similar manner, to find the coefficient of x^9 and that of higher powers in $Q(x)$. It is now evident that the details become increasingly complicated. Hence, it is preferable to calculate the coefficient for a given power by means of the appropriate recurrence relations. However, using the last of the three results occurring at the end of Section 3, it is possible to deduce the coefficient of x^{k-1} when k is even. The coefficient is

$$\frac{k}{k-1}\left\{1 + \frac{3(k-2)}{2(k-3)} + \frac{3\cdot 5(k-2)(k-4)}{2\cdot 4(k-3)(k-5)} + \frac{3\cdot 5\cdot 7(k-2)(k-4)(k-6)}{2\cdot 4\cdot 6(k-3)(k-5)(k-7)} + \cdots\right\},$$

the expression within the brackets terminating, since k is even.

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FIBONACCI RATIO IN A THERMODYNAMICAL CASE

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Consider the thermodynamics of an infinite chain of alternately spaced $2N$ molecules of donors and acceptors ($N \to \infty$), and assume there is an average of one mobile electron per molecule (as is quite common for some one-dimensional organic crystals [1, 2]).

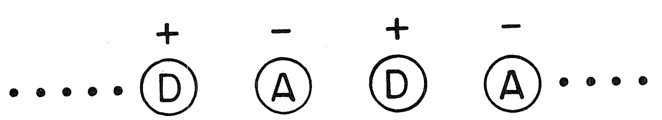

FIGURE 1

Each molecule may contain a maximum of two such electrons and as the temperature is raised two electrons may jump onto the same molecule. Because electrons repel each other, it costs an energy U_D or U_A to put two electrons on a molecule type D or type A, respectively; a common situation is that

$$U_D >> U_A.$$

Under these conditions, it can cost almost no energy to have sites A doubly occupied, while double occupancy of sites D is effectively eliminated.