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ELECTRONIC WAVE FUNCTIONS

XII. THE EVALUATION OF THE GENERAL VECTOR-COUPLING COEFFICIENTS BY AUTOMATIC COMPUTATION

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CONTENTS

A considerable number of different types of investigations on atomic and nuclear wave functions involve the use of vector-coupled functions and would be facilitated by an easy method of evaluation of the basic fundamental coefficients. This is particularly so for the present series of investigations, in which very complicated vector-coupled functions are used in convergent methods of atomic wave-function calculation. Hitherto the evaluation of these coefficients, which are independent of all aspects of a problem other than the irreducible representations of the rotational group concerned, has been extremely tedious while still requiring considerable mathematical understanding.

It has now been found possible to develop a method of calculation which can be performed purely automatically by the EDSAC, proceeding from the lowest argument values indefinitely through all higher values. A substantial table, which would otherwise require over a year of computation by a mathematician, has been obtained. This investigation constitutes a significant contribution to problems of wave-function calculation and also involves some minor innovations in the vector-coupling theory.

1. Introduction

Calculations on the wave functions of spherically symmetric systems, such as atoms and atomic nuclei, are generally regarded as involving very difficult mathematical theory. They involve the complexities of dealing with many-variable antisymmetric functions which are common to all accurate wave-function calculations, and also an extra complexity which arises because it is possible to achieve a much greater accuracy for the same amount of computation if the problem is formulated in terms of the conventional irreducible representations of the complete rotational group. For electronic wave functions of atoms the latter are the well-known eigenfunctions of the angular momentum operators $\mathbf{L}^2$, L_z, $\mathbf{S}^2$, S_z. The forms in which such eigenfunctions dependent on few variables are combined to give eigenfunctions dependent on many variables are conveniently described as vector-coupled functions, since the procedure corresponds exactly to the semi-physical vector-coupling process of combining approximate stationary states in the explanation of atomic

spectra. The only general method of reducing all integrals of the Schrödinger-Hamiltonian operating on such functions to relatively simple terms is that reported by Boys in parts IV to VI of this series. There it was shown that any integral could be progressively reduced in terms of certain coefficients denoted by U, V, W, Q and η, of which the Q and η can be disregarded from a computational point of view, since relatively few of these occur and their calculation is relatively simple. In the present investigation it has been found possible to devise a procedure to evaluate the U, V, W coefficients purely automatically and to construct a practical programme which performs this on the EDSAC, the electronic computation machine of the Mathematical Laboratory, Cambridge (see Wilkes 1949). This procedure causes values of U, V, W to be calculated in a definite sequence, so that any value is included if the sequence is continued sufficiently far. The procedure requires no external data and only necessitates starting, stopping and continuing at convenient times. This solution is thus a valuable complement to the general theory of the reduction of vector-coupled integrals.

In practical calculations the vector-coupled functions are frequently very complicated (see part XI), but this is due more to many repetitions of the vector-coupling process than to any inherent complexity. In essence, if it is suitable to use the direct products $A_m B_n$ of two sets of functions A_m and B_n which transform as irreducible representations of the rotational group to solve a given problem, then the routine calculation can generally be much reduced by using instead the linear combinations denoted by

$$\sum_m X(e, M, a, b, m)\, A_m B_{M-m} = AB\theta^{eM}, \tag{1}$$

where the X coefficients are defined so that these linear combinations themselves transform as irreducible representations of order e, with M labelling the particular elements. The orders of the A and B representations have been denoted by a and b, and the X coefficients depend only on the arguments shown. The set $AB\theta^{eM}$ is a typical vector-coupled set and can be further coupled with another connected set C_m to give the sets

$$AB\theta^{e}C\theta^{dM} = \sum_m X(d, M, e, c, m)\, AB\theta^{em}C_{M-m}. \tag{2}$$

If the other connected sets obtained by combining BC before joining to A are considered, then it can easily be shown (see part V) that the first sets are linear combinations of these, and that there are coefficients, here designated by U, such that

$$AB\theta^{e}C\theta^{dM} = \sum_f U\begin{pmatrix} a & b & c & d \\ e & & f & \end{pmatrix} A(BC\theta^{f})\,\theta^{dM}. \tag{3}$$

It is the calculation of these U coefficients which is the main problem of this investigation. The significance of these may perhaps be illustrated most definitely by considering an example in terms of ordinary spherical harmonics, although the actual range of application is, of course, much more general than this. If P'_m, D'_m and G'_m denote the sets of Tesseral harmonics of order 1, 2 and 4 respectively, then the vector couplings of these would satisfy

$$P'D'\theta^{3}G\theta^{5m} = \sum_f U\begin{pmatrix} 1 & 2 & 4 & 5 \\ 3 & & f & \end{pmatrix} P'(D'G'\theta^{f})\,\theta^{5m}. \tag{4}$$

In quantal investigations it is the integrals of the Hamiltonian operators on such vector-coupled functions which are required. The evaluation of integrals of these types have been considered in many rather complicated examinations, but probably the following particulars of important treatments serve to show the general development. Slater (1929) developed some particular methods of obtaining the final integral values for certain simple and particular symmetric cases by rather specialized methods which, however, avoid any detailed computation. Condon & Shortley (1935) describe more general methods in which large numbers of particular complicated relations occur. These might be regarded as implicitly equivalent to use of the foregoing X expansions, but although the methods were applicable to some complicated cases, they were restricted to rather symmetric integrals. Racah (1943 and earlier papers cited there) derived some more general and extremely complicated explicit formulas, but still left large classes of more unsymmetric integrals unconsidered. Boys (1951 *a*, *b*) formulated a scheme of evaluation of all integrals of the Schrödinger-Hamiltonian in terms of recurrence procedures involving the U, V, W, Q and η coefficients. It later became apparent that the U coefficients could be regarded as the essential quantities and the other coefficients expressed in terms of these.

The practical value of this adaptation to automatic computation is thus self-evident, but it is also interesting that this may be the first step towards developing procedures by which the whole problem of the reduction of vector-coupled integrals might be solved purely automatically. This would open up almost forbidden fields of physical problems to practical quantitative investigation, since these integral reductions constitute one of the great obstacles to such an investigation of structure of atoms in transition groups and calculations on complicated nuclear structure.

The special characteristics of the way in which the problem was formulated and the special analysis necessary for this automatic solution will now be described.

2. Notation

The essential property of the X coefficients and the five arguments on which these depend are shown by equation (1). It may be noted that $2e$, $2a$, $2b$, twice the arguments of $X(e, M, a, b, m)$, can only have positive integral values and that M and m are restricted by the conditions that m' for any irreducible representation $C_{m'}$ of order c can only take the values $-c$, $-c+1$, $-c+2$, ..., c. The explicit definition, removing all ambiguities of phase, etc., is complicated, and since only some special characteristics are used in the new way of evaluating the X coefficients described below, the definition stated fully in part IV will not be repeated here.

It may be noted that in the present analysis eigang values will be written either as suffixes or as function arguments, e.g. A_m or $A(m)$, solely as a matter of detailed convenience. This is consistent with the general theory in which a suffix is merely an argument restricted to a discrete set of values. For example, a U coefficient could be written as U_{ef}^{abcd} with six suffixes, but it is considered that a chain of reasoning can be followed more easily if the arguments are displayed out in a pattern corresponding to the functions with which they are associated, as in equation (3). The similar displays of the arguments of V and W are shown in equations (5) and (6).

The defining property of the U coefficients is given by equation (3). An explicit formula for these in terms of the X coefficients was given in part V, but a different formula, easier for computation but less symmetric, will be established and used here.

In part IV the W coefficients were defined in a way which was somewhat complicated but which corresponded closely to the way in which they are used. In theorem 8, part VI, it was shown that all the W values required for atomic wave-function calculations were given in terms of U coefficients by the formula of the following equation. It is now proposed to use this equation as a definition of W coefficients and to regard the cited theorem as showing that these satisfy the property required in their use, that is the original defining property. This appears to be a simpler approach than the original, although the definition now includes some ranges of values which never occur in atomic wave-function calculations. The W coefficients are thus defined by

$$W\begin{pmatrix} a & b \\ c & d \end{pmatrix} e\, f = U\begin{pmatrix} a & b & d \\ e & f & c \end{pmatrix} \mathrm{i}^{2(d-b-e)} \sqrt{\left(\frac{2f+1}{2e+1}\right)}. \tag{5}$$

It is similarly proposed to define the V coefficients by

$$V\begin{pmatrix} a & e \\ f & d \end{pmatrix} b\, c = U\begin{pmatrix} a & b & c \\ e & f & d \end{pmatrix} \mathrm{i}^{2(e-a)} \sqrt{\left(\frac{2c+1}{2f+1}\right)}. \tag{6}$$

The equivalence of this to the original definition of the V coefficients will be established in a series of theorems on another topic to be reported subsequently by S. F. B. No simple proof of this independently of a special examination of some integral values is known. Just as in the case of the W coefficients, it will probably be simplest to use this subsequently as a definition.

3. The scope and use of the progressive UVW table

The results which have been obtained by the automatic procedure to be reported here can be regarded as the first 2800 coefficient values of a general table in a rigidly prescribed pattern, which could in principle be continued indefinitely to include all possible U and W values and nearly all V values. These 2800 values have been generated purely automatically by the EDSAC. Since relatively few workers will actually be using such a table repeatedly, it has been considered suitable to deposit the whole table in the archives of the Royal Society and to reproduce here only the 560 U values. These are sufficient for casual reference, since all V and W values can be calculated from them by multiplication by square roots of simple fractions, which is negligibly simple compared with the procedure necessary to obtain the U values. For systematic use, especially since the coefficients are not generally used in a simple consecutive manner, it is very convenient to have full tables expressed in decimals. All the coefficients are square roots of fractions ranging up to such quantities as $\sqrt{(1375/7056)}$ towards the end of the present table, but the simple decimal form in which these have been evaluated is probably the most useful. Hitherto the coefficients have been used in calculations performed to 7 decimal figures to leave a margin over the 5 figures used in the final stages of the wave-function calculations. In accordance with this and matters of detailed convenience the results have been calculated to within about 1 in the 9th decimal place.

To describe the particulars of the calculation and the full results which are available the following description will be given in terms of the full table. The values given in the appendix are the arguments and U values of this.

There is a slight complexity in reading the required values from the table because, as has been shown in part VI, there are several equalities between coefficients with rearranged argument values, which make it possible to work with the special form of table described below, which is only about one-eighth as long as if all possible values were entered. As a result of this, it is necessary to perform certain rearrangements of arguments of desired coefficients before consulting the table.

Partly to state these complexities as precisely as possible and partly to provide a firm basis for explaining the number of other incidental and significant complexities of the subject, it appears simplest to begin with a categorical statement of the characteristics and use of the final table and to leave the justification and methods used until later.

The final table consists of unit entries, each containing five numerical values and corresponding to a particular set of values of the six arguments a, b, c, d, e, f. The values of $2a$, $2b$, ..., are tabulated on the right-hand side of the entry, which has the general form

$$\begin{array}{l} P\ \ p\ \ R\ \ r \\ Q\ \ q\ \ S\ \ s\ \ U \quad (2a),\ (2b),\ (2c),\ (2d),\ (2e),\ (2f), \end{array} \tag{7}$$

where P, Q, R, S are decimal fractions and p, q, r, s are integers 0 to 3. The entries are arranged in a straightforward numerico-alphabetic order so that a particular a, b, c, ..., set $x'_1, x'_2, \ldots$, occurs before another set $x''_1, x''_2, \ldots$, if there is an $x'_K < x''_K$ with all $x'_L = x''_L$ for $L < K$. Thus any particular set of values can be found by a procedure analogous to using a dictionary. For the reasons discussed below only certain restricted ranges of values of the arguments occur. The table, if continued sufficiently far, would contain any entry satisfying the following inequalities and none which does not satisfy them:

$$a > b > d; \quad a > c, \tag{8}$$

$$|a-b| \leqslant e \leqslant (a+b), \tag{9}$$

$$|c-d| \leqslant e \leqslant (c+d), \tag{10}$$

$$|b-c| \leqslant f \leqslant (b+c), \tag{11}$$

$$|a-d| \leqslant f \leqslant (a+d), \tag{12}$$

$$a, b, c, d > 0, \quad e, f \geqslant 0. \tag{13}$$

The values of $2a$, etc., are all integral and the differences in the inequalities (9), (10), (11) and (12) are all integral. It is convenient to refer in this text to a sequence of values a, b, c, d, e, f satisfying these conditions as a canonical sequence.

To find the value of a required coefficient $U(A, B, C, \ldots)$ it may be necessary to construct an equality

$$U\begin{pmatrix} A & B & C & D \\ E & F & & \end{pmatrix} = U\begin{pmatrix} a & b & c & d \\ e & f & & \end{pmatrix}, \tag{14}$$

according to the rules established in part VI where equality is proved when a, b, c, d is any rearrangement of A, B, C, D, in which neither A and C nor B and D are adjacent and in which $e = E$ if a, b are either A, B or C, D, but $e = F$ otherwise; and such that a, b, c, d, e, f is

a canonical arrangement. It is always possible to find such an arrangement and the required value is just the U value of the unit entry corresponding to a, b, c, d, e, f as shown above.

To find the value of a required coefficient

$$W\begin{pmatrix} A & B \\ C & D \end{matrix} E \; F\Big), \tag{15}$$

it is necessary to construct the a, b, c, d, e, f in which a, b, c, d is a canonical rearrangement of A, B, C, D and in which $e = E$ if a, b are on the same level as in (15) and $e = F$ if a, b are on different levels. If $e = E$ then the value

$$W\begin{pmatrix} d & c \\ a & b \end{matrix} e \; f\Big) = R\mathrm{i}^r \tag{16}$$

is read from the a, b, c, d, e, f entry of the table, and if $e = F$ the value

$$W\begin{pmatrix} c & b \\ d & a \end{matrix} f \; e\Big) = S\mathrm{i}^s. \tag{17}$$

If the W so evaluated has not an arrangement of arguments identical with that of the required W then this is easily obtained as ± 1 times the former by the symmetry relations

$$W\begin{pmatrix} A & B \\ C & D \end{matrix} E \; F\Big) = W\begin{pmatrix} C & D \\ A & B \end{matrix} E \; F\Big) \tag{18}$$

$$= W\begin{pmatrix} B & A \\ D & C \end{matrix} E \; F\Big)(-1)^{a+b-c-d}, \tag{19}$$

established in part IV.

To find the value of a required coefficient

$$V\begin{pmatrix} A & C & D \\ B & & E \end{matrix} F\Big), \tag{20}$$

it is necessary to examine whether one of the sequences

$$A \; C \; E \; F \; B \; D \quad \text{or} \quad B \; C \; D \; F \; A \; E, \quad \text{case (i)}$$

or

$$F \; A \; C \; E \; D \; B \quad \text{or} \quad F \; B \; C \; D \; E \; A, \quad \text{case (ii)}$$

satisfies the conditions for an a, b, c, d, e, f sequence. The last two symbols can always satisfy the conditions for e, f if the first four are satisfactory. In these cases the value of V can be read directly from the table, but otherwise, case (iii), the value must be calculated from a U coefficient by the relation described below. In case (i) the value

$$V\begin{pmatrix} A & C & D \\ B & & E \end{matrix} F\Big) = Q\mathrm{i}^q \tag{21}$$

for the entry corresponding to a, b, c, d, e, f is taken from the table. In case (ii) the value

$$V\begin{pmatrix} A & C & D \\ B & & E \end{matrix} F\Big) = P\mathrm{i}^p \tag{22}$$

corresponding to a, b, c, d, e, f is taken. In case (iii) it is necessary to use one of the relations

$$V\begin{pmatrix} A & C & D \\ B & & E \end{pmatrix} F = U\begin{pmatrix} A & C & E & F \\ B & & D & \end{pmatrix} \mathrm{i}^{2D-2A} \sqrt{\left(\frac{2E+1}{2B+1}\right)} \tag{23}$$

$$= U\begin{pmatrix} B & C & D & F \\ A & & E & \end{pmatrix} \mathrm{i}^{2E-2B} \sqrt{\left(\frac{2D+1}{2A+1}\right)}, \tag{24}$$

and to find the value of the U coefficient after any necessary rearrangement of the arguments as above.

It may be noted that it is theoretically possible for the coefficients to occur when one of the a, b, c, d is zero, although, as stated above, these cases have been omitted from the table. The reason for this omission is that $U = 1$ in all these cases (see part VI) and the values of V and W also follow very simply. Finally, it may be useful to illustrate the general use of the table by the following particular values which may be read from the entry shown:

P, Q	p, q	R, S	r, s	U	$(2a)$	$(2b)$	$(2c)$	$(2d)$	$(2e)$	$(2f)$
−0·866 025 405	3	−0·866 025 405	1							
−0·577 350 270	1	−0·577 350 270	3	−0·707 106 781	4	3	1	2	1	2

$$V\begin{pmatrix} \frac{3}{2} & \frac{1}{2} & 1 \\ \frac{1}{2} & & 1 \end{pmatrix} 2 = \mathrm{i}\sqrt{\tfrac{3}{2}}$$

$$V\begin{pmatrix} 2 & \frac{3}{2} & \frac{1}{2} \\ 1 & & \frac{1}{2} \end{pmatrix} 1 = -\mathrm{i}/\sqrt{3}$$

$$W\begin{pmatrix} 1 & \frac{1}{2} & \frac{1}{2} \\ 2 & \frac{3}{2} & \end{pmatrix} 1 = -\mathrm{i}\sqrt{\tfrac{3}{2}}$$

$$W\begin{pmatrix} \frac{1}{2} & \frac{3}{2} & 1 \\ 1 & 2 & \end{pmatrix} \tfrac{1}{2} = \mathrm{i}/\sqrt{3}$$

$$U\begin{pmatrix} 2 & \frac{3}{2} & \frac{1}{2} \\ \frac{1}{2} & 1 & \end{pmatrix} 1 = U\begin{pmatrix} \frac{1}{2} & \frac{3}{2} & 2 \\ 1 & & \frac{1}{2} \end{pmatrix} 1 = -1/\sqrt{2}$$

These rules provide a complete statement of the procedure for finding the value of any U, V or W coefficient from the general table. The justification of these rules depends on the method of evaluation of the tabulated quantities and the related theory. The method and theory for the U coefficients are complicated, but those for the derivation of the other tabulated quantities from the U coefficients are so simple that they can be explained immediately. This will be done here, and the remaining analysis for the U coefficient developed in § 4. The P, Q, etc., were computed from the argument values and the U value by the relations

$$P = U\sqrt{\left(\frac{2d+1}{2e+1}\right)}, \quad p = 2(f-b)+4n, \tag{25}$$

$$Q = U\sqrt{\left(\frac{2c+1}{2f+1}\right)}, \quad q = 2(e-a)+4n, \tag{26}$$

$$R = U\sqrt{\left(\frac{2f+1}{2e+1}\right)}, \quad r = 2(b-c-e)+4n, \tag{27}$$

$$S = U\sqrt{\left(\frac{2e+1}{2f+1}\right)}, \quad s = 2(a-b-f)+4n, \tag{28}$$

where n denotes the integer which in each case makes the values of p, q, r, s positive and less than 4.

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If the U value is assumed to be correct it follows from equations (5) and (27) and from the symmetry relations of the U coefficients that

$$Ri^r = U\begin{pmatrix} d & c & b & a \\ e & f \end{pmatrix}\sqrt{\left(\frac{2f+1}{2e+1}\right)}\,\mathrm{i}^{2b-2c-2e} = W\begin{pmatrix} d & c \\ a & b \end{pmatrix} e\, f\Big), \tag{29}$$

and similarly that $$Si^s = U\begin{pmatrix} d & a & b & c \\ f & e \end{pmatrix}\sqrt{\left(\frac{2e+1}{2f+1}\right)}\,\mathrm{i}^{2a-2b-2f} = W\begin{pmatrix} c & b \\ d & a \end{pmatrix} f\, e\Big), \tag{30}$$

which are just the functions whose values have been prescribed as given by Ri^r and Si^s. In the same way, from equations (6) and (25), it follows that

$$Pi^p = U\begin{pmatrix} b & c & d & a \\ f & e \end{pmatrix}\sqrt{\left(\frac{2d+1}{2e+1}\right)}\,\mathrm{i}^{2f-2b} = V\begin{pmatrix} b & c & f \\ e & d & a \end{pmatrix}, \tag{31}$$

and similarly that $$Qi^q = U\begin{pmatrix} a & b & c & d \\ e & f \end{pmatrix}\sqrt{\left(\frac{2c+1}{2f+1}\right)}\,\mathrm{i}^{2e-2a} = V\begin{pmatrix} a & b & e \\ f & c & d \end{pmatrix}, \tag{32}$$

again in accordance with the prescribed use of the general table. The other methods of use of the table are direct applications of the various symmetry properties established in part VI and of the definition relation (6).

The occurrence in the table of every U value, except the simple unity values mentioned above, is a consequence of the fact that all canonical arrangements of a, b, etc., are tabulated and that any desired value of U can be taken as equal to one of these by the symmetry relations. The form of the associated rules of obtaining required V and W values shows how any of these may be obtained directly or by a simple multiplication. These latter rules have been justified, and it merely remains to describe and justify the method of evaluation of the U coefficients.

4. The theory of the automatic computation procedures

The two essential stages in the calculation of the U coefficients are the calculation of the X coefficients and the calculation of each U coefficient in terms of these. The method used here for the second of these processes is related to the corresponding calculations in part VII, but the method used there for the X coefficients is not suitable for automatic computation since some of the X coefficients were only obtained in terms of long sequences of preceding values. This procedure is economical if considerable numbers of these values can be stored permanently, as in a calculation on paper, but is not economical in a machine with limited storage capacity, since a considerable sequence may have to be evaluated for any single required value. It was thus considered worth while examining the fundamental theory afresh to see if an alternative procedure could be found. This has been found possible by the following relations which provide a method of calculating a particular coefficient $X(L, M, a, b, m)$ when required without reference to the values of any other X coefficients.

Let $$y_m = X(L, M, a, b, m)/X(L, M, a, b, q), \tag{33}$$

where q is the maximum value of m for which an X coefficient exists with the given values of L, M, a, b. Let $A(m)$ and $B(m)$ be two connected sets of eigangs of the operators $\mathbf{L}_1$ and $\mathbf{L}_2$ respectively and with first eigang values a and b. Then since

$$\sum_m y_m A(m)\, B(M-m)$$

is a multiple of the derived vector-coupled set of eigangs with eigang values L and M it follows that

$$\begin{aligned}
&[L(L+1)-a(a+1)-b(b+1)]\sum_m y_m A(m)\,B(M-m)\\
&\quad=[(\boldsymbol{L}_1+\boldsymbol{L}_2)^2-\boldsymbol{L}_1^2-\boldsymbol{L}_2^2]\sum_m y_m A(m)\,B(M-m)\\
&\quad=[(L_{1x}+\mathrm{i}L_{1y})\,(L_{2x}-\mathrm{i}L_{2y})+(L_{1x}-\mathrm{i}L_{1y})\,(L_{2x}+\mathrm{i}L_{2y})+2L_{1z}L_{2z}]\\
&\qquad\times\sum_m y(m)\,A(m)\,B(M-m)\\
&\quad=\sum_m y_m A(m+1)\,B(M-m-1)\sqrt{[(a-m)\,(a+m+1)\,(b-M+m+1)\,(b+M-m)]}\\
&\qquad+\sum_m y_m A(m-1)\,B(M-m+1)\sqrt{[(a-m+1)\,(a+m)\,(b-M+m)\,(b+M-m+1)]}\\
&\qquad+\sum_m y_m A(m)\,B(M-m)\,[m(M-m)]\,2.
\end{aligned}\tag{34}$$

If this is written as one expression equated to zero, it is valid as shown in theorem 3, part IV, to equate the total coefficient of any particular eigang to zero. Thus it follows for each permissible value of m that

$$\alpha_m y_{m+1}+\beta_m y_m+\gamma_m y_{m-1}=0,\tag{35}$$

where

$$\left.\begin{aligned}
\alpha_m&=\sqrt{[(a-m+1)\,(a+m)\,(b-M+m)\,(b+M-m+1)]},\\
\beta_m&=a(a+1)+b(b+1)+2m(M-m)-L(L+1),\\
\gamma_m&=\sqrt{[(a-m)\,(a+m+1)\,(b-M+m+1)\,(b+M-m)]},
\end{aligned}\right\}\tag{36}$$

and the particular non-existing terms such as y_{q+1} are to be interpreted as zero.

The numerical evaluation of all the y_m in terms of the numerical values of the α_m, β_m, γ_m follows very simply by the recurrence procedure of evaluating each y_{m-1} in terms of y_m and y_{m+1} by the relation (35). The procedure can be begun directly since $y_q=1$ and $y_{q-1}=-\beta_q/\alpha_q$ by the equation (35) for $m=q$. If this procedure is continued to the lowest value of m and $y_{m'}$ and $\sum_m y_m^2$ evaluated, then it follows that

$$X(L,M,a,b,m')=y_{m'}/\sqrt{(\sum_m y_m^2)},\tag{37}$$

where the positive value of the square root is to be taken. This follows from the relations

$$\sum_m [X(L,M,a,b,m)]^2=1,\tag{38}$$

$$X(L,M,a,b,q)>0,\tag{39}$$

occurring in the fundamental definition in part IV and proved in part VI respectively. Hence the constant of proportionality between the X and y coefficients could only be as shown in (39).

The automatic subroutine which evaluated the X coefficients followed exactly this theory. For a given L, M, a, b, m' a minor sub-routine evaluated the α, β, γ coefficients as required and the y_m values were generated in turn. The sum $\sum_m y_m^2$ was generated as this proceeded and $y_{m'}$ stored when $m=m'$ was reached. Then at the end of the sequence the

required value was evaluated by equation (37). This method appears to be much simpler than any previously reported method for the evaluation of a particular X coefficient without reference to other values of X coefficients.

In part IV the U coefficients were defined in terms of a double summation of products of the X coefficients; in part VI a practical method of evaluation was used in which only a single summation was necessary but which involved certain rather arbitrary choices of terms; here another unsymmetric method dependent on a single summation is used, but this is expressed as the explicit formula (42). This is established by the following argument.

Let $A(m)$, $B(m)$, $C(m)$ be connected sets of eigangs with first eigang values a, b, c respectively. Consider the following two ways of expressing the same quantity:

$$AB\theta^{ee}C(d-e) = \sum_L X(L,d,e,c,e)\, AB\theta^{e}C\theta^{Ld}$$
$$= \sum_L \sum_f X(L,d,e,c,e)\, U\begin{pmatrix} a & b & c & L \\ e & f & & \end{pmatrix} A(BC\theta^{f})\,\theta^{Ld}, \qquad (40)$$

and

$$AB\theta^{ee}C(d-e) = \sum_m X(e,e,a,b,m)\, A(m)\, B(e-m)\, C(d-e)$$
$$= \sum_m \sum_f \sum_L X(e,e,a,b,m)\, X(f,d-m,b,c,e-m)\, X(L,d,a,f,m)\, A(BC\theta^{f})\,\theta^{Ld}. \qquad (41)$$

By theorem 3, part IV, it is possible to equate just the terms depending on the particular eigang $A(BC\theta^{f})\,\theta^{dd}$ and hence

$$U\begin{pmatrix} a & b & c & d \\ e & f & & \end{pmatrix} = \sum_m X(e,e,a,b,m)\, X(f,d-m,b,c,e-m)\, X(d,d,a,f,m)/X(d,d,e,c,e). \qquad (42)$$

The construction of an automatic programme to evaluate this, using the above X procedure as an ancillary subroutine, provided a number of difficulties, but these were chiefly of an arithmetical type, and it was finally found possible to make such a programme within the storage capacity of the EDSAC.

5. General characteristics of the automatic programmes

The requirements which caused most difficulty in the construction of the programme were the desirability of performing the arithmetical steps with sufficient accuracy to yield nearly 10 significant figures in the results and the limitation of the storage capacity to about 800 locations of 17 binary digits. It was not found possible to devise a programme to perform the whole calculation of the fundamental table described above and to be stored in this capacity. However, it was found possible to make two master programmes A and B, prepared in the usual manner as punched tapes, and requiring less than the available storage space. The effect of programme A was to generate from the output punch of the machine a tape C of unlimited length. In practice, successive portions of this were generated on separate occasions as convenient. The tape C carried sets of twelve quantities punched on it. These sets corresponded exactly to the canonical sets a, b, c, d, e, f and their order corresponded to the order of the latter in the final table of results. The first six symbols

were just the values $2a$, $2b$, $2c$, $2d$, $2e$, $2f$ from the canonical set, the next four symbols were the quantities p, q, r, s, whose occurrence in the final table has been described. The penultimate quantity was the maximum possible value of m occurring in formula (42) and the last quantity the total number of permissible values of m occurring in this formula.

On other occasions the programme B was read into the EDSAC and then, under the instructions of B, portions of tape C were read in as a basic data tape. The result of this was to generate another tape D which carried the final results and which when fed into a teleprinter gave the typed table with the same spatial arrangement as shown in the above example. The EDSAC generated tape C at approximately thirty complete entries per minute and tape D at about fifteen coefficient values per minute near the beginning of the table and three near the end.

The construction of the master programmes A and B was achieved by combining together numbers of subroutines performing simpler operations as described by Wilkes, Wheeler & Gill (1951). The details of these are too extensive to report here, but the following particulars illustrate the nature of the difficulties. If the contents of the storage locations are regarded as representing numbers less than unity, it was necessary in the calculation of the X coefficients to work with the quantities $y_m 2^{-16}$, since the y_m could become large as the sequence was constructed. On the other hand, these were required with a significant accuracy of at least 2^{-34} to give final results accurate to 10 decimal places, and it was thus necessary to use over 50 binary digits to represent the working numbers. This necessitated the use of two long storage locations, equivalent to four short locations, for each number. It was then necessary to perform the arithmetical operations on these double-length numbers by special subroutines which were modifications of some constructed previously by Dr V. E. Price.

On the other hand, the generation of the canonical sets of values in programme A was a completely different kind of problem. This was solved by the construction of a subroutine of a more general type than was required for this particular problem. This was constructed to order the sets of values of any number of variables $a_1, a_2, \ldots, a_n$ taking only integral values. The subroutine was applicable to the case when any variable a_r could assume all values from a'_r to a''_r, these being dependent on the values of $a_{r-1}, a_{r-2}, \ldots, a_1$. The first step in forming the next combination of the sequence was the examination whether a_n had achieved its maximum value consistent with the values of the other variables. If the value was not the maximum, this was increased to the next value; but if it was the maximum, the subroutine then examined a_{n-1} and behaved exactly as at the previous stage. This process was continued until a variable not at its maximum value was found, when the subroutine increased this and placed all the variables previously examined at their minimum values. This subroutine will probably be of value in arranging other complicated systems of functions and was of immediate application for obtaining the canonical sets. The permissible ranges of each of f, e, d, c, b, a were specified in terms of the following variables by the inequalities of equations (8) to (13). Hence every time the subroutine was obeyed the next canonical set was generated.

Considerable co-ordination of the various processes in the calculation of the X coefficients and in the combination of these to give the U coefficients was necessary and, apart from the main points referred to above, the programme construction consisted chiefly of a rather long and tedious combination of all the detailed processes.

6. Discussion

In involved calculations of this type it is highly desirable to have some check which can be performed directly on the final copy of the table so that any copying or mechanical error as well as errors in the calculation may be detected. The main check used here consisted of the confirmation on a desk machine that the U coefficients for a given set of a, b, c, d values form an orthogonal matrix, that is

$$\sum_f U\begin{pmatrix} a & b & c & d \\ e & & & f \end{pmatrix} U\begin{pmatrix} a & b & c & d \\ g & & & f \end{pmatrix} = \delta(e, g). \tag{43}$$

Every tabulated U value was used in this way in at least one check relation. The V and W coefficients were checked by direct relations of § 3.

The work involved in the construction of a programme of the present type is considerable, but once this has been done no further problems arise until this has been applied to reach values for which either the storage capacity is insufficient or the time taken becomes impracticable. Even in these cases the limit can frequently be extended by fresh devices only requiring the modification of relatively small parts of the programme.

It should be noted that it is not necessary to calculate all values consecutively. If some particular high value is required at an early occasion the programme can be started just below this.

It is not very easy to estimate the time taken to calculate the table by ordinary means, but this would probably require an effort lasting over a year and involving considerable mental attention. The actual time taken by the EDSAC was not more than a few nights.

Finally, it may be noted that the nature of any calculation of such coefficients is nearly of the type which would be regarded as mathematical rather than arithmetical since so many particular relations and inequalities are involved. It is hoped that this constitutes a first step towards the construction of automatic programmes for other calculations in this field which at the present time would be regarded as essentially theoretical.

The authors would like to acknowledge their gratitude and indebtedness to Dr M. V. Wilkes and members of the Mathematical Laboratory, Cambridge, for assistance and for placing the resources of the laboratory at the authors' disposal; and to Dr V. E. Price for many suggestions on the programmes. R. C. S. is also indebted to the Royal Commission for the Exhibition of 1851 for the award of a scholarship during the tenure of which this investigation was carried out.

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Appendix. The general sequence of UVW vector-coupling coefficients

(2a)	(2b)	(2c)	(2d)	(2e)	(2f)	U
1	1	1	1	0	0	−0·5
1	1	1	1	0	2	0·866 025 403
1	1	1	1	2	0	0·866 025 403
1	1	1	1	2	2	0·5
2	1	2	1	1	1	−0·333 333 333
2	1	2	1	1	3	0·942 809 041
2	1	2	1	3	1	0·942 809 041
2	1	2	1	3	3	0·333 333 333
2	2	1	1	0	1	−0·577 350 270
2	2	1	1	0	3	0·816 496 581
2	2	1	1	2	1	0·816 496 581
2	2	1	1	2	3	0·577 350 269
2	2	2	2	0	0	0·333 333 333
2	2	2	2	0	2	−0·577 350 270
2	2	2	2	0	4	0·745 355 992
2	2	2	2	2	0	−0·577 350 270
2	2	2	2	2	2	0·5
2	2	2	2	2	4	0·645 497 224
2	2	2	2	4	0	0·745 355 992
2	2	2	2	4	2	0·645 497 224
2	2	2	2	4	4	0·166 666 667
3	1	1	1	2	2	1·0
3	1	3	1	2	2	−0·25
3	1	3	1	2	4	0·968 245 836
3	1	3	1	4	2	0·968 245 836
3	1	3	1	4	4	0·25
3	2	1	2	1	1	−0·666 666 667
3	2	1	2	1	3	0·745 355 992
3	2	1	2	3	1	0·745 355 992
3	2	1	2	3	3	0·666 666 667
3	2	2	1	1	2	−0·408 248 291
3	2	2	1	1	4	0·912 870 929
3	2	2	1	3	2	0·912 870 929
3	2	2	1	3	4	0·408 248 290
3	2	3	2	1	1	0·166 666 667
3	2	3	2	1	3	−0·471 404 521
3	2	3	2	1	5	0·866 025 403
3	2	3	2	3	1	−0·471 404 521
3	2	3	2	3	3	0·733 333 333
3	2	3	2	3	5	0·489 897 948
3	2	3	2	5	1	0·866 025 403
3	2	3	2	5	3	0·489 897 948
3	2	3	2	5	5	0·1
3	3	1	1	0	2	−0·612 372 437
3	3	1	1	0	4	0·790 569 414
3	3	1	1	2	2	0·790 569 414
3	3	1	1	2	4	0·612 372 435
3	3	1	3	2	2	−0·5
3	3	1	3	2	4	0·866 025 403
3	3	1	3	4	2	0·866 025 403
3	3	1	3	4	4	0·5
3	3	2	2	0	1	0·408 248 290
3	3	2	2	0	3	−0·577 350 270
3	3	2	2	0	5	0·707 106 781
3	3	2	2	2	1	−0·645 497 225
3	3	2	2	2	3	0·365 148 371
3	3	2	2	2	5	0·670 820 393
3	3	2	2	4	1	0·645 497 224
3	3	2	2	4	3	0·730 296 743
3	3	2	2	4	5	0·223 606 797
3	3	3	1	2	2	−0·5
3	3	3	1	2	4	0·866 025 403
3	3	3	1	4	2	0·866 025 403
3	3	3	1	4	4	0·5
3	3	3	3	0	0	−0·25
3	3	3	3	0	2	0·433 012 701
3	3	3	3	0	4	−0·559 016 995
3	3	3	3	0	6	0·661 437 828
3	3	3	3	2	0	0·433 012 702
3	3	3	3	2	2	−0·55
3	3	3	3	2	4	0·193 649 167
3	3	3	3	2	6	0·687 386 353
3	3	3	3	4	0	−0·559 016 995
3	3	3	3	4	2	0·193 649 167
3	3	3	3	4	4	0·75
3	3	3	3	4	6	0·295 803 989
3	3	3	3	6	0	0·661 437 828
3	3	3	3	6	2	0·687 386 353
3	3	3	3	6	4	0·295 803 989
3	3	3	3	6	6	0·05
4	1	1	2	3	2	1·0
4	1	4	1	3	3	−0·2
4	1	4	1	3	5	0·979 795 897
4	1	4	1	5	3	0·979 795 897
4	1	4	1	5	5	0·2
4	2	2	2	2	2	−0·5
4	2	2	2	2	4	0·866 025 403
4	2	2	2	4	2	0·866 025 403
4	2	2	2	4	4	0·5
4	2	3	1	2	3	−0·316 227 767
4	2	3	1	2	5	0·948 683 298
4	2	3	1	4	3	0·948 683 298
4	2	3	1	4	5	0·316 227 765
4	2	4	2	2	2	0·1
4	2	4	2	2	4	−0·387 298 335
4	2	4	2	2	6	0·916 515 139
4	2	4	2	4	2	−0·387 298 335
4	2	4	2	4	4	0·833 333 333
4	2	4	2	4	6	0·394 405 318
4	2	4	2	6	2	0·916 515 139
4	2	4	2	6	4	0·394 405 318
4	2	4	2	6	6	0·066 666 666
4	3	1	2	1	2	−0·707 106 781
4	3	1	2	1	4	0·707 106 781
4	3	1	2	3	2	0·707 106 781
4	3	1	2	3	4	0·707 106 781
4	3	2	1	1	3	−0·447 213 596
4	3	2	1	1	5	0·894 427 190

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Appendix (*cont.*)

(2*a*)	(2*b*)	(2*c*)	(2*d*)	(2*e*)	(2*f*)	*U*
4	3	2	1	3	3	0·894 427 190
4	3	2	1	3	5	0·447 213 595
4	3	2	3	1	1	0·5
4	3	2	3	1	3	−0·632 455 533
4	3	2	3	1	5	0·591 607 978
4	3	2	3	3	1	−0·632 455 533
4	3	2	3	3	3	0·2
4	3	2	3	3	5	0·748 331 476
4	3	2	3	5	1	0·591 607 978
4	3	2	3	5	3	0·748 331 476
4	3	2	3	5	5	0·3
4	3	3	2	1	2	0·223 606 797
4	3	3	2	1	4	−0·5
4	3	3	2	1	6	0·836 660 026
4	3	3	2	3	2	−0·565 685 425
4	3	3	2	3	4	0·632 455 532
4	3	3	2	3	6	0·529 150 262
4	3	3	2	5	2	0·793 725 393
4	3	3	2	5	4	0·591 607 978
4	3	3	2	5	6	0·141 421 356
4	3	4	1	3	3	−0·4
4	3	4	1	3	5	0·916 515 139
4	3	4	1	5	3	0·916 515 139
4	3	4	1	5	5	0·4
4	3	4	3	1	1	−0·1
4	3	4	3	1	3	0·282 842 712
4	3	4	3	1	5	−0·519 615 243
4	3	4	3	1	7	0·8
4	3	4	3	3	1	0·282 842 712
4	3	4	3	3	3	−0·6
4	3	4	3	3	5	0·489 897 948
4	3	4	3	3	7	0·565 685 424
4	3	4	3	5	1	−0·519 615 242
4	3	4	3	5	3	0·489 897 948
4	3	4	3	5	5	0·671 428 571
4	3	4	3	5	7	0·197 948 663
4	3	4	3	7	1	0·8
4	3	4	3	7	3	0·565 685 424
4	3	4	3	7	5	0·197 948 663
4	3	4	3	7	7	0·028 571 428
4	4	1	1	0	3	−0·632 455 533
4	4	1	1	0	5	0·774 596 668
4	4	1	1	2	3	0·774 596 668
4	4	1	1	2	5	0·632 455 533
4	4	1	3	2	3	−0·547 722 558
4	4	1	3	2	5	0·836 660 026
4	4	1	3	4	3	0·836 660 026
4	4	1	3	4	5	0·547 722 557
4	4	2	2	0	2	0·447 213 595
4	4	2	2	0	4	−0·577 350 270
4	4	2	2	0	6	0·683 130 051
4	4	2	2	2	2	−0·670 820 394
4	4	2	2	2	4	0·288 675 134
4	4	2	2	2	6	0·683 130 051
4	4	2	2	4	2	0·591 607 978
4	4	2	2	4	4	0·763 762 615
4	4	2	2	4	6	0·258 198 889
4	4	2	4	2	2	0·3
4	4	2	4	2	4	−0·591 607 979
4	4	2	4	2	6	0·748 331 476
4	4	2	4	4	2	−0·591 607 979
4	4	2	4	4	4	0·5
4	4	2	4	4	6	0·632 455 532
4	4	2	4	6	2	0·748 331 476
4	4	2	4	6	4	0·632 455 532
4	4	2	4	6	6	0·2
4	4	3	1	2	3	−0·547 722 558
4	4	3	1	2	5	0·836 660 026
4	4	3	1	4	3	0·836 660 026
4	4	3	1	4	5	0·547 722 557
4	4	3	3	0	1	−0·316 227 767
4	4	3	3	0	3	0·447 213 595
4	4	3	3	0	5	−0·547 722 558
4	4	3	3	0	7	0·632 455 532
4	4	3	3	2	1	0·519 615 242
4	4	3	3	2	3	−0·489 897 949
4	4	3	3	2	5	0·1
4	4	3	3	2	7	0·692 820 323
4	4	3	3	4	1	−0·591 607 979
4	4	3	3	4	3	0·0
4	4	3	3	4	5	0·731 925 054
4	4	3	3	4	7	0·338 061 701
4	4	3	3	6	1	0·529 150 262
4	4	3	3	6	3	0·748 331 476
4	4	3	3	6	5	0·392 792 202
4	4	3	3	6	7	0·075 592 894
4	4	4	2	2	2	0·3
4	4	4	2	2	4	−0·591 607 979
4	4	4	2	2	6	0·748 331 476
4	4	4	2	4	2	−0·591 607 979
4	4	4	2	4	4	0·5
4	4	4	2	4	6	0·632 455 532
4	4	4	2	6	2	0·748 331 476
4	4	4	2	6	4	0·632 455 532
4	4	4	2	6	6	0·2
4	4	4	4	0	0	0·2
4	4	4	4	0	2	−0·346 410 162
4	4	4	4	0	4	0·447 213 595
4	4	4	4	0	6	−0·529 150 263
4	4	4	4	0	8	0·6
4	4	4	4	2	0	−0·346 410 162
4	4	4	4	2	2	0·5
4	4	4	4	2	4	−0·387 298 335
4	4	4	4	2	6	0·0
4	4	4	4	2	8	0·692 820 323
4	4	4	4	4	0	0·447 213 595
4	4	4	4	4	2	−0·387 298 335
4	4	4	4	4	4	−0·214 285 715
4	4	4	4	4	6	0·676 123 403
4	4	4	4	4	8	0·383 325 938
4	4	4	4	6	0	−0·529 150 263
4	4	4	4	6	2	0·0
4	4	4	4	6	4	0·676 123 403
4	4	4	4	6	6	0·5

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Appendix (*cont.*)

(2*a*)	(2*b*)	(2*c*)	(2*d*)	(2*e*)	(2*f*)	*U*
4	4	4	4	6	8	0·113 389 341
4	4	4	4	8	0	0·6
4	4	4	4	8	2	0·692 820 323
4	4	4	4	8	4	0·383 325 938
4	4	4	4	8	6	0·113 389 341
4	4	4	4	8	8	0·014 285 714
5	1	1	3	4	2	1·0
5	1	3	1	4	4	1·0
5	1	5	1	4	4	−0·166 666 667
5	1	5	1	4	6	0·986 013 297
5	1	5	1	6	4	0·986 013 297
5	1	5	1	6	6	0·166 666 666
5	2	2	1	3	4	1·0
5	2	3	2	3	3	−0·4
5	2	3	2	3	5	0·916 515 139
5	2	3	2	5	3	0·916 515 139
5	2	3	2	5	5	0·4
5	2	4	1	3	4	−0·258 198 890
5	2	4	1	3	6	0·966 091 782
5	2	4	1	5	4	0·966 091 782
5	2	4	1	5	6	0·258 198 889
5	2	5	2	3	3	0·066 666 666
5	2	5	2	3	5	−0·326 598 633
5	2	5	2	3	7	0·942 809 041
5	2	5	2	5	3	−0·326 598 633
5	2	5	2	5	5	0·885 714 285
5	2	5	2	5	7	0·329 914 439
5	2	5	2	7	3	0·942 809 041
5	2	5	2	7	5	0·329 914 439
5	2	5	2	7	7	0·047 619 047
5	3	1	1	2	4	1·0
5	3	1	3	2	2	−0·75
5	3	1	3	2	4	0·661 437 828
5	3	1	3	4	2	0·661 437 828
5	3	1	3	4	4	0·75
5	3	2	2	2	3	−0·547 722 558
5	3	2	2	2	5	0·836 660 026
5	3	2	2	4	3	0·836 660 026
5	3	2	2	4	5	0·547 722 557
5	3	3	1	2	4	−0·353 553 391
5	3	3	1	2	6	0·935 414 346
5	3	3	1	4	4	0·935 414 346
5	3	3	1	4	6	0·353 553 390
5	3	3	3	2	2	0·3
5	3	3	3	2	4	−0·591 607 979
5	3	3	3	2	6	0·748 331 476
5	3	3	3	4	2	−0·591 607 979
5	3	3	3	4	4	0·5
5	3	3	3	4	6	0·632 455 532
5	3	3	3	6	2	0·748 331 476
5	3	3	3	6	4	0·632 455 532
5	3	3	3	6	6	0·2
5	3	4	2	2	3	0·141 421 356
5	3	4	2	2	5	−0·424 264 069
5	3	4	2	2	7	0·894 427 190
5	3	4	2	4	3	−0·483 045 892
5	3	4	2	4	5	0·759 072 115
5	3	4	2	4	7	0·436 435 780
5	3	4	2	6	3	0·864 098 759
5	3	4	2	6	5	0·493 770 719
5	3	4	2	6	7	0·097 590 007
5	3	5	1	4	4	−0·333 333 333
5	3	5	1	4	6	0·942 809 041
5	3	5	1	6	4	0·942 809 041
5	3	5	1	6	6	0·333 333 333
5	3	5	3	2	2	−0·05
5	3	5	3	2	4	0·193 649 167
5	3	5	3	2	6	−0·458 257 570
5	3	5	3	2	8	0·866 025 403
5	3	5	3	4	2	0·193 649 167
5	3	5	3	4	4	−0·559 523 810
5	3	5	3	4	6	0·647 951 595
5	3	5	3	4	8	0·479 157 423
5	3	5	3	6	2	−0·458 257 570
5	3	5	3	6	4	0·647 951 595
5	3	5	3	6	6	0·591 666 666
5	3	5	3	6	8	0·141 736 677
5	3	5	3	8	2	0·866 025 403
5	3	5	3	8	4	0·479 157 423
5	3	5	3	8	6	0·141 736 677
5	3	5	3	8	8	0·017 857 142
5	4	1	2	1	3	−0·730 296 744
5	4	1	2	1	5	0·683 130 051
5	4	1	2	3	3	0·683 130 051
5	4	1	2	3	5	0·730 296 743
5	4	1	4	3	3	−0·6
5	4	1	4	3	5	0·8
5	4	1	4	5	3	0·8
5	4	1	4	5	5	0·6
5	4	2	1	1	4	−0·471 404 521
5	4	2	1	1	6	0·881 917 104
5	4	2	1	3	4	0·881 917 104
5	4	2	1	3	6	0·471 404 520
5	4	2	3	1	2	0·547 722 557
5	4	2	3	1	4	−0·623 609 565
5	4	2	3	1	6	0·557 773 350
5	4	2	3	3	2	−0·648 074 070
5	4	2	3	3	4	0·105 409 255
5	4	2	3	3	6	0·754 247 233
5	4	2	3	5	2	0·529 150 262
5	4	2	3	5	4	0·774 596 668
5	4	2	3	5	6	0·346 410 161
5	4	3	2	1	3	0·258 198 889
5	4	3	2	1	5	−0·516 397 780
5	4	3	2	1	7	0·816 496 580
5	4	3	2	3	3	−0·611 010 093
5	4	3	2	3	5	0·567 366 514
5	4	3	2	3	7	0·552 052 447
5	4	3	2	5	3	0·748 331 476
5	4	3	2	5	5	0·641 426 980
5	4	3	2	5	7	0·169 030 851
5	4	3	4	1	1	−0·4

PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES

Appendix (*cont.*)

(2*a*)	(2*b*)	(2*c*)	(2*d*)	(2*e*)	(2*f*)	*U*
5	4	3	4	1	3	0·529 150 262
5	4	3	4	1	5	−0·565 685 425
5	4	3	4	1	7	0·489 897 948
5	4	3	4	3	1	0·529 150 262
5	4	3	4	3	3	−0·4
5	4	3	4	3	5	−0·106 904 497
5	4	3	4	3	7	0·740 656 079
5	4	3	4	5	1	−0·565 685 425
5	4	3	4	5	3	−0·106 904 497
5	4	3	4	5	5	0·685 714 285
5	4	3	4	5	7	0·445 384 493
5	4	3	4	7	1	0·489 897 948
5	4	3	4	7	3	0·740 656 079
5	4	3	4	7	5	0·445 384 493
5	4	3	4	7	7	0·114 285 714
5	4	4	1	3	4	−0·447 213 596
5	4	4	1	3	6	0·894 427 190
5	4	4	1	5	4	0·894 427 190
5	4	4	1	5	6	0·447 213 595
5	4	4	3	1	2	−0·141 421 356
5	4	4	3	1	4	0·316 227 765
5	4	4	3	1	6	−0·529 150 263
5	4	4	3	1	8	0·774 596 668
5	4	4	3	3	2	0·374 165 738
5	4	4	3	3	4	−0·597 614 306
5	4	4	3	3	6	0·4
5	4	4	3	3	8	0·585 540 044
5	4	4	3	5	2	−0·6
5	4	4	3	5	4	0·319 438 282
5	4	4	3	5	6	0·694 879 228
5	4	4	3	5	8	0·234 738 239
5	4	4	3	7	2	0·692 820 323
5	4	4	3	7	4	0·663 940 002
5	4	4	3	7	6	0·277 746 031
5	4	4	3	7	8	0·045 175 395
5	4	5	2	3	3	0·2
5	4	5	2	3	5	−0·523 722 937
5	4	5	2	3	7	0·828 078 670
5	4	5	2	5	3	−0·523 722 937
5	4	5	2	5	5	0·657 142 857
5	4	5	2	5	7	0·542 104 741
5	4	5	2	7	3	0·828 078 670
5	4	5	2	7	5	0·542 104 741
5	4	5	2	7	7	0·142 857 143
5	4	5	4	1	1	0·066 666 666
5	4	5	4	1	3	−0·188 561 808
5	4	5	4	1	5	0·346 410 161
5	4	5	4	1	7	−0·533 333 333
5	4	5	4	1	9	0·745 355 992
5	4	5	4	3	1	−0·188 561 808
5	4	5	4	3	3	0·447 619 047
5	4	5	4	3	5	−0·559 883 370
5	4	5	4	3	7	0·296 311 413
5	4	5	4	3	9	0·602 338 602
5	4	5	4	5	1	0·346 410 161
5	4	5	4	5	3	−0·559 883 370
5	4	5	4	5	5	0·1
5	4	5	4	5	7	0·692 820 323
5	4	5	4	5	9	0·276 641 667
5	4	5	4	7	1	−0·533 333 333
5	4	5	4	7	3	0·296 311 413
5	4	5	4	7	5	0·692 820 323
5	4	5	4	7	7	0·377 777 777
5	4	5	4	7	9	0·070 986 284
5	4	5	4	9	1	0·745 355 992
5	4	5	4	9	3	0·602 338 602
5	4	5	4	9	5	0·276 641 667
5	4	5	4	9	7	0·070 986 284
5	4	5	4	9	9	0·007 936 508
5	5	1	1	0	4	−0·645 497 225
5	5	1	1	0	6	0·763 762 615
5	5	1	1	2	4	0·763 762 615
5	5	1	1	2	6	0·645 497 224
5	5	1	3	2	4	−0·577 350 270
5	5	1	3	2	6	0·816 496 580
5	5	1	3	4	4	0·816 496 580
5	5	1	3	4	6	0·577 350 269
5	5	1	5	4	4	−0·5
5	5	1	5	4	6	0·866 025 403
5	5	1	5	6	4	0·866 025 403
5	5	1	5	6	6	0·5
5	5	2	2	0	3	0·471 404 520
5	5	2	2	0	5	−0·577 350 270
5	5	2	2	0	7	0·666 666 666
5	5	2	2	2	3	−0·683 130 052
5	5	2	2	2	5	0·239 045 721
5	5	2	2	2	7	0·690 065 559
5	5	2	2	4	3	0·557 773 350
5	5	2	2	4	5	0·780 720 058
5	5	2	2	4	7	0·281 718 084
5	5	2	4	2	3	0·346 410 161
5	5	2	4	2	5	−0·604 743 157
5	5	2	4	2	7	0·717 137 165
5	5	2	4	4	3	−0·632 455 533
5	5	2	4	4	5	0·414 039 335
5	5	2	4	4	7	0·654 653 670
5	5	2	4	6	3	0·692 820 323
5	5	2	4	6	5	0·680 336 051
5	5	2	4	6	7	0·239 045 721
5	5	3	1	2	4	−0·577 350 270
5	5	3	1	2	6	0·816 496 580
5	5	3	1	4	4	0·816 496 580
5	5	3	1	4	6	0·577 350 269
5	5	3	3	0	2	−0·353 553 391
5	5	3	3	0	4	0·456 435 464
5	5	3	3	0	6	−0·540 061 726
5	5	3	3	0	8	0·612 372 435
5	5	3	3	2	2	0·561 248 608
5	5	3	3	2	4	−0·448 542 615
5	5	3	3	2	6	0·040 824 828
5	5	3	3	2	8	0·694 365 074
5	5	3	3	4	2	−0·591 607 979
5	5	3	3	4	4	−0·109 108 946
5	5	3	3	4	6	0·710 046 946
5	5	3	3	4	8	0·365 962 527

PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES

Appendix (*cont.*)

(2*a*)	(2*b*)	(2*c*)	(2*d*)	(2*e*)	(2*f*)	*U*
5	5	3	3	6	2	0·458 257 569
5	5	3	3	6	4	0·760 638 829
5	5	3	3	6	6	0·45
5	5	3	3	6	8	0·094 491 118
5	5	3	5	2	2	−0·2
5	5	3	5	2	4	0·414 039 335
5	5	3	5	2	6	−0·6
5	5	3	5	2	8	0·654 653 670
5	5	3	5	4	2	0·414 039 335
5	5	3	5	4	4	−0·571 428 572
5	5	3	5	4	6	0·207 019 667
5	5	3	5	4	8	0·677 630 926
5	5	3	5	6	2	−0·6
5	5	3	5	6	4	0·207 019 667
5	5	3	5	6	6	0·7
5	5	3	5	6	8	0·327 326 835
5	5	3	5	8	2	0·654 653 670
5	5	3	5	8	4	0·677 630 926
5	5	3	5	8	6	0·327 326 835
5	5	3	5	8	8	0·071 428 571
5	5	4	2	2	3	0·346 410 161
5	5	4	2	2	5	−0·604 743 157
5	5	4	2	2	7	0·717 137 165
5	5	4	2	4	3	−0·632 455 533
5	5	4	2	4	5	0·414 039 335
5	5	4	2	4	7	0·654 653 670
5	5	4	2	6	3	0·692 820 323
5	5	4	2	6	5	0·680 336 051
5	5	4	2	6	7	0·239 045 721
5	5	4	4	0	1	0·258 198 889
5	5	4	4	0	3	−0·365 148 372
5	5	4	4	0	5	0·447 213 595
5	5	4	4	0	7	−0·516 397 780
5	5	4	4	0	9	0·577 350 269
5	5	4	4	2	1	−0·432 049 381
5	5	4	4	2	3	0·480 079 358
5	5	4	4	2	5	−0·320 713 491
5	5	4	4	2	7	−0·061 721 341
5	5	4	4	2	9	0·690 065 559
5	5	4	4	4	1	0·516 397 779
5	5	4	4	4	3	−0·260 820 266
5	5	4	4	4	5	−0·319 438 283
5	5	4	4	4	7	0·627 054 446
5	5	4	4	4	9	0·412 393 049
5	5	4	4	6	1	−0·529 150 263
5	5	4	4	6	3	−0·213 808 994
5	5	4	4	6	5	0·589 188 303
5	5	4	4	6	7	0·554 347 893
5	5	4	4	6	9	0·140 859 042
5	5	4	4	8	1	0·447 213 595
5	5	4	4	8	3	0·722 806 322
5	5	4	4	8	5	0·497 955 002
5	5	4	4	8	7	0·170 367 084
5	5	4	4	8	9	0·023 809 524
5	5	5	1	4	4	−0·5
5	5	5	1	4	6	0·866 025 403
5	5	5	1	6	4	0·866 025 403
5	5	5	1	6	6	0·5
5	5	5	3	2	2	−0·2
5	5	5	3	2	4	0·414 039 335
5	5	5	3	2	6	−0·6
5	5	5	3	2	8	0·654 653 670
5	5	5	3	4	2	0·414 039 335
5	5	5	3	4	4	−0·571 428 572
5	5	5	3	4	6	0·207 019 667
5	5	5	3	4	8	0·677 630 926
5	5	5	3	6	2	−0·6
5	5	5	3	6	4	0·207 019 667
5	5	5	3	6	6	0·7
5	5	5	3	6	8	0·327 326 835
5	5	5	3	8	2	0·654 653 670
5	5	5	3	8	4	0·677 630 926
5	5	5	3	8	6	0·327 326 835
5	5	5	3	8	8	0·071 428 571
5	5	5	5	0	0	−0·166 666 667
5	5	5	5	0	2	0·288 675 134
5	5	5	5	0	4	−0·372 677 997
5	5	5	5	0	6	0·440 958 552
5	5	5	5	0	8	−0·5
5	5	5	5	0	(10)	0·552 770 798
5	5	5	5	2	0	0·288 675 134
5	5	5	5	2	2	−0·442 857 143
5	5	5	5	2	4	0·424 183 890
5	5	5	5	2	6	−0·240 039 680
5	5	5	5	2	8	−0·123 717 915
5	5	5	5	2	(10)	0·683 876 505
5	5	5	5	4	0	−0·372 677 997
5	5	5	5	4	2	0·424 183 890
5	5	5	5	4	4	−0·083 333 333
5	5	5	5	4	6	−0·408 491 224
5	5	5	5	4	8	0·559 016 994
5	5	5	5	4	(10)	0·441 440 385
5	5	5	5	6	0	0·440 958 552
5	5	5	5	6	2	−0·240 039 680
5	5	5	5	6	4	−0·408 491 223
5	5	5	5	6	6	0·438 888 888
5	5	5	5	6	8	0·598 443 748
5	5	5	5	6	(10)	0·174 106 436
5	5	5	5	8	0	−0·5
5	5	5	5	8	2	−0·123 717 915
5	5	5	5	8	4	0·559 016 994
5	5	5	5	8	6	0·598 443 748
5	5	5	5	8	8	0·25
5	5	5	5	8	(10)	0·039 483 628
5	5	5	5	(10)	0	0·552 770 798
5	5	5	5	(10)	2	0·683 876 505
5	5	5	5	(10)	4	0·441 440 385
5	5	5	5	(10)	6	0·174 106 436
5	5	5	5	(10)	8	0·039 483 628
5	5	5	5	(10)	(10)	0·003 968 253