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Continued fraction solutions to systems of linear equations

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Abstract. Solutions of systems of linear equations or linear recurrence relations are obtained in the form of series of products of continued fractions. Simple rules are presented for obtaining the series for any given problem. The continued fraction expansion is superior to ordinary perturbation theory; each continued fraction represents a partial summation of the ordinary perturbation series. The use of the method in eigenvalue problems, and its possible application in numerical analysis, is discussed.

1. Introduction

A continued fraction formalism of the quantum mechanical eigenvalue problem and of the theory of scattering processes has been given by Feenberg (1948a, b) who also discussed its relation to the Rayleigh–Schrödinger and Wigner–Brillouin perturbation series (Feenberg 1958). Different methods of obtaining Feenberg's results were described by Richards (1948) and Feshbach (1948) (see also Morse and Feshbach 1953). Independently, continued fraction expressions for the transition probabilities in quantum mechanical systems were given by Swain (1975a, to be referred to as I), where a diagrammatic interpretation of the solutions was also described (note that this treatment includes the solution to the eigenvalue problem), and by Gontier *et al* (1975). A recent paper dealing with the application of continued fraction methods to the calculation of thermodynamic Green functions has been published by Bowen (1975). Here, as in I, we do not discuss questions of convergence, but we note that Masson (1970) has proved a theorem which assures the convergence of the continued fraction solutions for an extremely wide class of Hamiltonians (see also Bowen 1975).

Previously, the majority of applications of continued fraction methods have been of a formal nature, perhaps because the complexity of the summation restrictions in the solutions has discouraged their use in specific problems. However, a feature of the treatment given in I is that rather than direct substitution into these complicated expressions, the use of a simple set of rules is advocated which may be used to write down the solutions to any specified order. In fact, these rules are simpler than those used in modern quantum field theory (e.g. Abrikosov *et al* 1963). Examples of the application of this method to specific problems in quantum optics have already been given in I, Swain (1975b), and McClean and Swain (1976).

In this paper we demonstrate that continued fraction solutions of this type may be found generally to systems of linear equations, whether in matrix equation or difference

equation form, and that they are suitable both for analytic or numerical computation. Of course, the previously described solutions to quantum mechanical problems are a special case of this general treatment.

One area in which continued fraction solutions to linear three-term recurrence relations have proved very useful recently is the study of the behaviour of two-level atoms in oscillating electromagnetic fields (e.g. Autler and Townes 1955, Stenholm 1972, Swain 1973a, b, Stenholm and Aminoff 1973, Tsukada and Ogawa 1973, Swain 1974). These three-term recurrence relations may be solved by elementary methods, and the application of the more general methods to be described is not essential. The continued fraction solutions are more useful than ordinary perturbation solutions in that they are valid at high field strengths or in the vicinity of a resonance. For example, in Swain (1974) the perturbation series for the three-quantum resonance is apparently divergent at high field strengths, whereas a low-order truncation to the continued fraction solution gives the position of the resonance accurately over the whole range of field strengths. However, several authors (Stenholm 1972, Tsukada *et al* 1974) have commented on the difficulty of obtaining solutions of a similar type for more general conditions (multi-level atoms, non-orthogonal fields, etc). The methods to be described in this paper may be applied straightforwardly to such situations. *We give simple rules for obtaining solutions to systems of linear equations or linear difference equations of arbitrary order.* Such systems are manifestly of very frequent occurrence in theoretical physics. We emphasize again that this approach is much superior to ordinary perturbation theory; the continued fractions may be considered to be obtained by summing certain terms of the ordinary perturbation series to all orders.

In § 2 we consider the problem of obtaining the solution to a system of linear inhomogeneous equations in matrix form. The solutions are founded on general expansions for a determinant and its complementary minors. In § 3 we consider the form of the solutions when the linear equations are in difference equation form. Rules for obtaining the solutions in both cases are given in § 4. In § 5, the problem of homogeneous linear equations is considered.

2. Inversion of the matrix equations

We consider first of all the problem of finding the N variables x_j, $j = 1, 2, \ldots N$ where these variables satisfy the N linearly independent equations

$$\sum_{j=1}^{N} a_{ij}x_j = b_j, \qquad i = 1, 2, \ldots, N. \tag{1}$$

(If necessary, N may be allowed to approach infinity.) The elements a_{ij} form a square matrix whose determinant we denote by A ($A \neq 0$). The formal solution to this problem is given in books on linear algebra (see e.g. Margenau and Murphy 1956) and may be written as

$$x_j = \sum_{k=1}^{N} (-1)^{j+k} \frac{b_k A^{kj}}{A}, \qquad j = 1, 2, \ldots, N. \tag{2}$$

where A^{kj} is the determinant which is obtained from A by removing the kth row and jth column.

In order to obtain a continued fraction expression for x_j we need to make use of the relations

$$A = a_{jj}\mathscr{A}^{j} - \sum_{\alpha\neq j} a_{j\alpha}a_{\alpha j}\mathscr{A}^{\alpha,j} + \sum_{\alpha\neq j}\sum_{\beta\neq\alpha,j} a_{j\alpha}a_{\alpha\beta}a_{\beta j}\mathscr{A}^{\alpha,\beta,j} - \sum_{\alpha\neq j}\sum_{\beta\neq\alpha,j}\sum_{\gamma\neq\alpha,\beta,j} a_{j\alpha}a_{\alpha\beta}a_{\beta\gamma}a_{\gamma j}\mathscr{A}^{\alpha,\beta,\gamma,j} + \ldots \tag{3}$$

and, for $k \neq j$,

$$A^{kj} = (-1)^{k+j-1}\left(a_{jk}\mathscr{A}^{j,k} - \sum_{\alpha\neq j,k} a_{j\alpha}a_{\alpha j}\mathscr{A}^{\alpha,j,k} + \sum_{\alpha\neq j,k}\sum_{\beta\neq\alpha,j,k} a_{j\alpha}a_{\alpha\beta}a_{\beta k}\mathscr{A}^{\alpha,\beta,j,k} + \ldots\right) \tag{4}$$

where $\mathscr{A}^{\alpha,\beta,\ldots,\nu}$ denotes the determinant obtained from A by removing the αth, the βth, ... and the νth rows and columns. Clearly the order in which the superscripts $\alpha, \beta, \ldots, \nu$ in $\mathscr{A}^{\alpha,\beta,\ldots,\nu}$ are written is of no significance. Expressions (3) and (4) may be established by repeated use of the Cauchy expansion of a determinant (see e.g. Aitken 1956). The sums over $\alpha, \beta, \ldots$ etc extend from 1 to N, but this has not been written in explicitly. Expressions (3) and (4) give the expansion of a determinant in terms of determinants of successively lower orders. Note that $\mathscr{A}^{1,2,3,\ldots,N} \equiv 1$.

On substituting from (4) into (2) we obtain

$$x_j = \frac{b_j\mathscr{A}^{j}}{A} - \sum_{k\neq j}\left(\frac{a_{jk}\mathscr{A}^{j,k}}{A} - \sum_{\alpha\neq j,k} a_{j\alpha}a_{\alpha j}\frac{\mathscr{A}^{\alpha,j,k}}{A} + \ldots\right)b_k. \tag{5}$$

In order to manipulate this into a form suitable for obtaining approximate solutions it is convenient to introduce the $\mathscr{D}$ functions by the definitions

$$\mathscr{D}_j \equiv \frac{A}{\mathscr{A}^{j}}, \qquad \mathscr{D}_{\nu}^{\alpha,\beta,\ldots,\mu} \equiv \frac{\mathscr{A}^{\alpha,\beta,\ldots,\mu}}{\mathscr{A}^{\alpha,\beta,\ldots,\mu,\nu}}. \tag{6}$$

From the expression (3) we can obtain an expansion for $\mathscr{D}_j$:

$$\mathscr{D}_j = a_{jj} - \sum_{\alpha\neq j}\frac{a_{j\alpha}a_{\alpha j}}{\mathscr{D}_{\alpha}^{j}} + \sum_{\alpha\neq j}\sum_{\beta\neq\alpha,j}\frac{a_{j\alpha}a_{\alpha\beta}a_{\beta j}}{\mathscr{D}_{\alpha}^{j}\mathscr{D}_{\beta}^{\alpha j}} - \sum_{\alpha\neq j}\sum_{\beta\neq\alpha,j}\sum_{\gamma\neq\alpha,\beta,j}\frac{a_{j\alpha}a_{\alpha\beta}a_{\beta j}}{\mathscr{D}_{\alpha}^{j}\mathscr{D}_{\beta}^{\alpha j}\mathscr{D}_{\gamma}^{\alpha\beta j}} + \ldots \tag{7}$$

where we have made use of relations of the type

$$\frac{\mathscr{A}^{j}}{\mathscr{A}^{\alpha,\beta,\gamma,j}} = \frac{\mathscr{A}^{j}}{\mathscr{A}^{\alpha j}}\frac{\mathscr{A}^{\alpha,j}}{\mathscr{A}^{\alpha,\beta,j}}\frac{\mathscr{A}^{\alpha,\beta,j}}{\mathscr{A}^{\alpha,\beta,\gamma,j}} \equiv \mathscr{D}_{\alpha}^{j}\mathscr{D}_{\beta}^{\alpha,j}\mathscr{D}_{\gamma}^{\alpha,\beta,j}. \tag{8}$$

However, we note that this decomposition is not unique; we could have written

$$\frac{\mathscr{A}^{j}}{\mathscr{A}^{\alpha,\beta,\gamma,j}} = \frac{\mathscr{A}^{j}}{\mathscr{A}^{\beta,j}}\frac{\mathscr{A}^{\beta,j}}{\mathscr{A}^{\beta,\gamma,j}}\frac{\mathscr{A}^{\beta,\gamma,j}}{\mathscr{A}^{\alpha,\beta,\gamma,j}} = \mathscr{D}_{\beta}^{j}\mathscr{D}_{\gamma}^{\beta,j}\mathscr{D}_{\alpha}^{\beta,\gamma,j} \tag{9}$$

or in fact any permutation of the subscripts α, β, γ providing that the superscripts are changed accordingly. However, at a later stage, in order to give an interpretation of the formulae, we will find it convenient to define a standard order. An expansion for $\mathscr{D}_{\nu}^{\alpha,\beta,\ldots,\mu}$ is easily obtained from (7) (with $j = \nu$) by observing that, in addition to the νth row and column being excluded, the αth, βth, ... and νth rows and columns are also excluded. Consequently,

$$\mathscr{D}_{\nu}^{\alpha,\beta,\ldots,\mu} = a_{\nu\nu} - \sum_{\xi\neq\alpha\beta\ldots\mu\nu}\frac{a_{\nu\xi}a_{\xi\nu}}{\mathscr{D}_{\xi}^{\alpha\beta\ldots\mu\nu}} + \sum_{\xi\neq\alpha\beta\ldots\nu}\sum_{0\neq\alpha\beta\ldots\nu\xi}\frac{a_{\nu\xi}a_{\xi 0}a_{0\nu}}{\mathscr{D}_{\xi}^{\alpha\beta\ldots\nu}\mathscr{D}_{0}^{\alpha\beta\ldots\nu\xi}} + \ldots \tag{10}$$

We note that we could achieve a simpler notation by omitting the conditions on the sums providing it is understood that no terms are allowed to appear in which the subscript of any $\mathscr{D}$ function is equal to any of the superscripts of that $\mathscr{D}$ function. We indicate this restriction by starring the sums (cf Feenberg 1948a).

Making use of expressions similar to (8) in (5) we finally obtain the expansion

$$x_j = \frac{b_j}{\mathscr{D}_j} - \sum_k^* b_k \left(\frac{a_{jk}}{\mathscr{D}_j \mathscr{D}_k^j} - \sum_\alpha^* \frac{a_{j\alpha} a_{\alpha k}}{\mathscr{D}_j \mathscr{D}_\alpha^j \mathscr{D}_k^{\alpha j}} + \sum_\alpha^* \sum_\beta^* \frac{a_{j\alpha} a_{\alpha\beta} a_{\beta k}}{\mathscr{D}_j \mathscr{D}_\alpha^j \mathscr{D}_\beta^{\alpha j} \mathscr{D}_k^{\alpha\beta j}} + \ldots \right). \tag{11}$$

An explicit expression for a $\mathscr{D}$ function (say $\mathscr{D}_j$), may be obtained by repeatedly using expression (10) in expression (7). The result is that the $\mathscr{D}$ functions in general may be expressed as the sums of products of continued fractions. For a finite value of N, the series for the $\mathscr{D}$ functions given in (10) and (7) and for x_j given in (11) terminate, and the resulting expressions are exact. However, if N is infinite, the series and continued fractions are also infinite, and usually approximations have to be introduced to terminate them and so obtain approximate solutions. Examples of such truncation procedures as applied to quantum mechanical problems have been given in I, Swain (1974, 1975b), and McClean and Swain (1976).

The expressions (7), (10) and (11) for the solutions are undeniably complicated, this perhaps being the reason why continued fraction methods have not been applied as widely as they might and it is preferable to introduce procedures other than direct substitution to obtain the solutions such as the set of rules given in I for the case of time-dependent quantum mechanical perturbation theory. However, before we do this it is convenient to look first at the problem of linear difference equations, as the method of treatment is closely analogous to that given in the preceding discussion.

3. The difference equations

We consider a set of $(2\nu+1)$-term linear inhomogeneous difference equations of the form

$$\sum_{j=-\nu}^{+\nu} c_j(i) x_{i+j} = b_i \tag{12}$$

where i may take on all negative and positive integer values, or perhaps the positive integer values only, when we set $x_l = 0$ for $l \leqslant 0$. (Expression (12) is quite general; to treat a four-term difference equation for example we may set $\nu = 2$ and take $c_{-2}(i) = 0$, all i.) The correspondence with the matrix equation (1) (for N infinite) is most obvious for the case where i takes on only positive integer values. If we set $i+j \to j$, then (12) may be written in the form (1) if

$$a_{ij} = \begin{cases} c_{j-i}(i); & j = i-\nu, i-\nu+1, \ldots i+\nu-1, i+\nu \\ 0; & j < i-\nu \quad \text{or} \quad j > i+\nu. \end{cases} \tag{13}$$

From (11), the general solution may be written as

$$x_j = \frac{b_j}{\mathscr{D}_j} - \sum_\alpha^* \frac{b_{j+\alpha} c_\alpha(j)}{\mathscr{D}_j \mathscr{D}_{j+\alpha}^j} + \sum_\alpha^* \sum_\beta^* \frac{b_{j+\alpha+\beta} c_\alpha(j) c_\beta(j+\alpha)}{\mathscr{D}_j \mathscr{D}_{j+\alpha}^j \mathscr{D}_{j+\alpha+\beta}^{j,j+\alpha}}$$

$$- \sum_\alpha^* \sum_\beta^* \sum_\gamma^* \frac{b_{j+\alpha+\beta+\gamma} c_\alpha(j) c_\beta(j+\alpha) c_\gamma(j+\alpha+\beta)}{\mathscr{D}_j \mathscr{D}_{j+\alpha}^j \mathscr{D}_{j+\alpha+\beta}^{j,j+\alpha} \mathscr{D}_{j+\alpha+\beta+\gamma}^{j,j+\alpha,j+\alpha+\beta}} + \ldots \tag{14}$$

with the $\mathscr{D}$ functions given by, e.g.

$$\mathscr{D}^{j,j+\alpha}_{j+\alpha+\beta} = c_0(j+\alpha+\beta) - \sum_\gamma{}^* \frac{c_\gamma(j+\alpha+\beta)c_{-\gamma}(j+\alpha+\beta+\gamma)}{\mathscr{D}^{j,j+\alpha,j+\alpha+\beta}_{j+\alpha+\beta+\gamma}}$$

$$+\sum_\gamma{}^* \sum_\delta{}^* \frac{c_\gamma(j+\alpha+\beta)c_\delta(j+\alpha+\beta+\gamma)c_{-(\gamma+\delta)}(j+\alpha+\beta+\gamma+\delta)}{\mathscr{D}^{j,j+\alpha,j+\alpha+\beta}_{j+\alpha+\beta+\gamma}\mathscr{D}^{j,j+\alpha,j+\alpha+\beta,j+\alpha+\beta+\gamma}_{j+\alpha+\beta+\gamma+\delta}} + \ldots \quad (15)$$

Note that the solutions (14) and (15) which we have just obtained are the ones which satisfy

$$x_j \to \frac{b_j}{c_0(j)} \qquad \text{as } c_i(j) \to 0 \quad \text{for } i \neq 0, \quad (16)$$

so that these solutions are particularly useful if the 'off-diagonal' elements $c_i(j), i \neq 0$, are small compared to the diagonal elements $c_0(j)$.

4. Rules for obtaining the solutions

Rather than substituting into the complicated expressions (10), (11), (14) and (15) for the x_j it is much simpler to develop a set of rules which give the solution directly. It is convenient to introduce the suggestive terms 'state' for the subscripts—e.g. the suffix k in x_k is referred to as the state k, and 'transition strength' for the off-diagonal matrix elements a_{ij} between states i and j (or $c_k(j)$ for transitions between states $j+k$ and j in the difference equation case).

To consider how to interpret the equations let us put $j = 1$ in (11) and consider the first few terms

$$x_1 = \frac{b_1}{\mathscr{D}_1} - \left(\frac{b_2a_{21}}{\mathscr{D}_1\mathscr{D}_2^1} + \frac{b_3a_{31}}{\mathscr{D}_1\mathscr{D}_3^1} + \ldots\right) + \left(\frac{b_3a_{32}a_{21}}{\mathscr{D}_1\mathscr{D}_2^1\mathscr{D}_3^{12}} + \frac{b_4a_{42}a_{21}}{\mathscr{D}_1\mathscr{D}_2^1\mathscr{D}_4^{12}} + \ldots\right) + \ldots . \quad (17)$$

We may interpret this equation in the following way: the first contribution to x_1, $b_1/\mathscr{D}_1$, is comprised of the 'probability', b_1, that the system is initially in the state 1 times the probability that it remains there, $\mathscr{D}_1^{-1}$. Hence $\mathscr{D}_1^{-1}$ may be considered as a kind of propagator for the state 1. The second term is comprised of the probability that the system is initially in the state 2 (state 3, etc) times the probability that under the influence of the 'interaction' (whose strength is measured by the off-diagonal element a_{21}) the system makes a transition from state 2 to state 1 (state 3, etc to state 1). Between the times when the interaction acts the system propagates in states 2 and then state 1. Similarly, the third term represents the probability that the system was initially in state 3 times the probability that it ends up in state 1 by proceeding through the intermediate state 2.

Thus it is convenient to picture the various contributions to x_j as arising from *processes* by which the system proceeds from one state to another under the influence of the 'interaction'. Thus for x_1, the processes shown explicitly in (17) would be

$$\begin{array}{llll} \overset{b_2}{2} & \xrightarrow{a_{21}} 1, & \overset{b_3}{3} \xrightarrow{a_{31}} 1, \ldots & \text{first order} \\ \mathscr{D}_2^1 \quad \mathscr{D}_1 & & \mathscr{D}_3^1 \quad \mathscr{D}_1 & \end{array}$$

$$\begin{array}{llll} \overset{b_3}{3} & \xrightarrow{a_{32}} 2 \xrightarrow{a_{21}} 1, & \overset{b_4}{4} \xrightarrow{a_{42}} 2 \xrightarrow{a_{21}} 1, \ldots & \text{second order} \\ \mathscr{D}_3^{1,2} \quad \mathscr{D}_2^1 \quad \mathscr{D}_1 & & \mathscr{D}_4^{1,2} \quad \mathscr{D}_2^1 \quad \mathscr{D}_1 & \end{array}$$

and so on. It is natural to associate the transition strengths a_{ij}, propagators $\mathscr{D}_j$ and initial weightings b_k as shown in the diagrams. Note that the only processes which contribute to x_j are those in which the states are all different. Such processes we shall refer to as *irreducible*. (We allow the possibility of the initial and final states being the same.) The order of a process is defined to be the number of times a transition strength appears in that process.

Consider now the $\mathscr{D}$ functions (for example $\mathscr{D}_3^{1,4}$). From (10) the first few contributions are

$$\mathscr{D}_3^{1,4} = a_{33} - \frac{a_{32}a_{23}}{\mathscr{D}_2^{1,3,4}} - \frac{a_{35}a_{53}}{\mathscr{D}_5^{1,3,4}} - \ldots + \frac{a_{32}a_{25}a_{53}}{\mathscr{D}_2^{1,3,4}\mathscr{D}_5^{1,2,3,4}} + \frac{a_{32}a_{26}a_{63}}{\mathscr{D}_2^{1,3,4}\mathscr{D}_6^{1,2,3,4}} + \ldots . \tag{18}$$

Apart from the first term, these contributions may be considered as arising from the processes

$$3 \xrightarrow{a_{32}} \underset{\mathscr{D}_2^{1,3,4}}{2} \xrightarrow{a_{23}} 3, \qquad 3 \xrightarrow{a_{35}} \underset{\mathscr{D}_5^{1,3,4}}{5} \xrightarrow{a_{53}} 3, \ldots$$

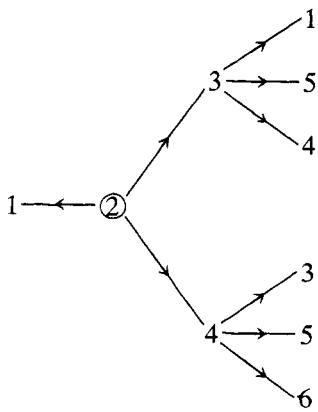
$$3 \xrightarrow{a_{32}} \underset{\mathscr{D}_2^{1,3,4}}{2} \xrightarrow{a_{25}} \underset{\mathscr{D}_5^{1,2,3,4}}{5} \xrightarrow{a_{53}} 3, \qquad 3 \xrightarrow{a_{35}} \underset{\mathscr{D}_2^{1,3,4}}{2} \xrightarrow{a_{26}} \underset{\mathscr{D}_6^{1,2,3,4}}{6} \xrightarrow{a_{63}} 3, \ldots .$$

A very similar interpretation may be given for the difference equation case, if now the interaction strength between two states $k \to l$ is taken to be $c_{l-k}(k)$.

Hence we formulate the following rules for obtaining solutions to linear equations.

Rule 1. The series for x_j

(*a*) Write down all the states which are connected irreducibly to the state j up to and including the order being considered. Thus for a five-term difference equation, with $x_l = 0$ for $l \leqslant 0$, the state j is connected to states $j \pm 1$, $j \pm 2$ so that for $j = 2$ the tree diagram including processes up to second order is



(19)

(*b*) with each transition $k \to l$ associate the interaction strength a_{kl} (or $c_{l-k}(k)$ for difference equations).

(*c*) With each state m in a process associate the factor $1/\mathscr{D}_m^{j\ldots l}$ where the states $j, \ldots, l$ are the ones which precede m in the process.

(*d*) With the terminal state n associate the factor b_n.

For each process, take the product of all these factors, together with the factor $(-1)^K$ where K is the order of the process, and add the contributions of all the processes considered to the zero-order contribution $b_j/\mathscr{D}_j$. Thus the contributions of the first-order processes shown in (19) are

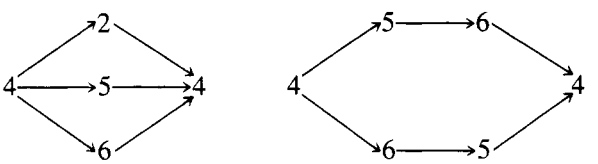
$$\begin{array}{lll} b_1 & b_3 & b_4 \\ 1 \xrightarrow[\mathscr{D}_1^2]{c_{-1}(2)} 2, & 3 \xrightarrow[\mathscr{D}_3^2]{c_1(2)} 2, & 4 \xrightarrow[\mathscr{D}_4^2]{c_2(2)} 2 \\ \dfrac{-1\,.\,c_{-1}(2)}{\mathscr{D}_2\mathscr{D}_1^2} & \dfrac{-1\,.\,c_1(2)}{\mathscr{D}_2\mathscr{D}_3^2} & \dfrac{-1\,.\,c_2(2)}{\mathscr{D}_2\mathscr{D}_4^2} \end{array} \tag{20}$$

and the contributions of the second-order processes may be similarly calculated. Hence the diagram (19) gives the following expression for x_2:

$$\begin{aligned} x_2 = \frac{b_2}{\mathscr{D}_2} - \frac{1}{\mathscr{D}_2}\left(\frac{b_1c_{-1}(2)}{\mathscr{D}_1^2} + \frac{b_3c_1(2)}{\mathscr{D}_3^2} + \frac{b_4c_2(4)}{\mathscr{D}_4^2}\right) \\ + \frac{1}{\mathscr{D}_2}\left(\frac{b_1c_{-2}(3)c_1(2)}{\mathscr{D}_3^2\mathscr{D}_1^{2,3}} + \frac{b_5c_2(3)c_1(2)}{\mathscr{D}_3^2\mathscr{D}_5^{2,3}} + \frac{b_4c_1(3)c_1(2)}{\mathscr{D}_3^2\mathscr{D}_4^{2,3}}\right. \\ \left. + \frac{b_3c_2(2)c_{-1}(4)}{\mathscr{D}_4^2\mathscr{D}_3^{2,4}} + \frac{b_5c_2(2)c_1(4)}{\mathscr{D}_4^2\mathscr{D}_5^{2,4}} + \frac{b_6c_2(2)c_2(4)}{\mathscr{D}_4^2\mathscr{D}_6^{2,4}}\right). \end{aligned} \tag{21}$$

Rule 2. The series for $\mathscr{D}_m^{j\ldots l}$

(*a*) To calculate the Kth order contribution to $\mathscr{D}_m^{j\ldots l}$ write down all the irreducible, *exclusive* processes which take one from the state m through $(k-1)$ intermediate states and back to the state m. An *exclusive* process for $\mathscr{D}_m^{j\ldots l}$ is one in which the states $j, \ldots, l$ which appear as superscripts are *not* allowed to participate. Referring again to our example of the five-term difference equation, the second- and third-order contributions to e.g. $\mathscr{D}_4^{1,3}$ are



(22)

Note that the conditions of exclusivity and irreducibility greatly reduce the number of third-order processes.

(*b*) With each transition $k \to l$ associate the factor a_{kl} (or $c_{l-k}(k)$), and with each *intermediate state* r (i.e. excluding initial and final state) associate the factor $1/\mathscr{D}_r^{j\ldots lmn\ldots q}$ where the states $n \ldots q$ are the ones which precede r in the process. Taking the product of all these factors together with $(-1)^{K+1}$ gives the contribution of a process. The contributions of all the second-, third-, ..., Kth-order contributions are then added to the zeroth-order contribution a_{mm} (or $c_0(m)$).

Thus the diagrams (22) lead to the expression

$$\mathscr{D}_4^{1,3} = c_0(4) - \frac{c_2(2)c_{-2}(4)}{\mathscr{D}_2^{1,3,4}} - \frac{c_{-1}(5)c_1(4)}{\mathscr{D}_5^{1,3,4}} - \frac{c_{-2}(6)c_2(4)}{\mathscr{D}_6^{1,3,4}} + \frac{c_{-1}(5)c_{-1}(6)c_2(4)}{\mathscr{D}_5^{1,3,4}\mathscr{D}_6^{1,3,4,5}} + \frac{c_{-2}(6)c_1(5)c_1(4)}{\mathscr{D}_6^{1,3,4}\mathscr{D}_5^{1,3,4,6}}. \tag{23}$$

The $\mathscr{D}$ functions which appear in the denominators of expression (23) may be similarly calculated to some specified order using rule 2.

We do not give further examples of applications of these rules here, as applications in the special case of quantum mechanical problems have been discussed in I, Swain (1975b) and McClean and Swain (1976). Also the continued fraction solutions obtained in e.g. Autler and Townes (1955), Stenholm (1972), Stenholm and Aminoff (1973), Tsukada and Ogawa (1973), and Smithers and Lu (1974) may be written down very easily by straightforward application of these rules.

A comment on the possible application of this method to numerical calculations is in order. In the great majority of problems which deal with matrices of relatively low order, one wants *all* the components of the vector $\boldsymbol{x}$ which is the solution of (1). For such a calculation, the present method would be inferior to conventional methods, such as Gaussian elimination (see e.g. Fox 1964), for although it has the advantages that the elements of the matrix are not changed at each step of the calculation, and there are no problems analogous to the choice of pivot, the continued fraction method gives only one particular component, x_j—say, of the solution $\boldsymbol{x}$. The situation is different if, for example, the matrix is a function of a parameter, ξ, and one wants to calculate a particular $x_j(\xi)$ for several values of this parameter. The present method is then more economical than the conventional ones. For such an application as this, the matrix involved is likely to be large and sparse—and in this circumstance the continued fraction expressions would be particularly simple. Large, sparse matrices frequently arise when a problem has been expressed in difference equation form.

The method could be used for an infinite matrix if, say, the off-diagonal elements were sufficiently small compared to the diagonal ones to ensure convergence of x_j. Then the series and continued fractions in the solutions (11) or (14) could be truncated at a stage appropriate to a pre-determined accuracy for x_j.

5. Homogeneous linear equations

Consider the set of linear homogeneous equations

$$\sum_j d_{ij} y_j = 0, \qquad i = 1, 2, \ldots . \tag{24}$$

If we divide each equation in the set by one of the y's—say y_k, then we obtain

$$\sum_{j \neq k} d_{ij}(y_i/y_k) = -d_{ik}, \qquad i = 1, 2, \ldots . \tag{25}$$

This is of the same form as (1) if we set

$$a_{ij} = \begin{cases} d_{ij}; & j \neq k \\ 0; & j = k \end{cases} \qquad x_i = y_i/y_k, \qquad b_i = -d_{ik} \tag{26}$$

and so we can solve for the ratios y_i/y_k using the rules described in § 4. However, the solutions obtained will only be consistent if

$$\det a_{ij} \equiv A = 0. \tag{27}$$

If the zeros of $\mathscr{A}^j$ do not occur at the same positions of those of A, expression (26) is equivalent to $A/\mathscr{A}^j = 0$, or, using the expansion (3), to

$$\mathscr{D}_j \equiv a_{jj} - \sum_\alpha{}^* \frac{a_{j\alpha}a_{\alpha j}}{\mathscr{D}^j_\alpha} + \sum_\alpha{}^* \sum_\beta{}^* \frac{a_{j\alpha}a_{\alpha\beta}a_{\beta j}}{\mathscr{D}^j_\alpha \mathscr{D}^{\alpha,j}_\beta} + \ldots . \tag{28}$$

An important class of problems of this type is the eigenvalue problem,

$$\det(a_{ij} - \lambda\delta_{ij}) = 0 \tag{29}$$

or, using the expansion (27),

$$a_{jj} - \lambda - \sum_\alpha{}^* \frac{a_{j\alpha}a_{\alpha j}}{\mathscr{D}^j_\alpha(\lambda)} + \sum_\alpha{}^* \sum_\beta{}^* \frac{a_{j\alpha}a_{\alpha\beta}a_{\beta j}}{\mathscr{D}^j_\alpha(\lambda)\mathscr{D}^{\alpha,j}_\beta(\lambda)} + \ldots = 0 \tag{30}$$

where the $\mathscr{D}(\lambda)$'s are obtained from the corresponding $\mathscr{D}$ functions by replacing every diagonal element a_{ll} by $a_{ll} - \lambda$.

Expression (30) provides the basis of a numerical method for determining eigenvalues. For example, consider

$$\begin{vmatrix} a_{11}-\lambda & a_{12} & a_{13} & \ldots \\ a_{21} & a_{22}-\lambda & a_{23} & \ldots \\ a_{31} & a_{32} & a_{33}-\lambda & \ldots \\ \ldots & \ldots & \ldots & \end{vmatrix} = 0. \tag{31}$$

In many problems, the diagonal elements will be much larger than the off-diagonal elements, in which case a zeroth approximation to the eigenvalues is

$$\lambda_j = a_{jj}, \qquad j = 1, 2, \ldots . \tag{32}$$

Suppose we wanted a value for the eigenvalue near $\lambda_1 \simeq a_{11}$. Then from (30), we have

$$\begin{aligned} a_{11} - \lambda - \cfrac{a_{12}a_{21}}{a_{22}-\lambda - \cfrac{a_{23}a_{32}}{a_{33}-\lambda - \ldots}} - \cfrac{a_{13}a_{31}}{a_{33}-\lambda - \cfrac{a_{32}a_{23}}{a_{22}-\lambda - \ldots}} - \ldots \\ + \cfrac{a_{12}a_{23}a_{31}}{\left(a_{22}-\lambda - \cfrac{a_{23}a_{32}}{a_{33}-\lambda-\ldots} - \ldots\right)\left(a_{33}-\lambda - \cfrac{a_{34}a_{43}}{a_{44}-\lambda-\ldots} - \ldots\right)} \\ + \cfrac{a_{13}a_{32}a_{21}}{\left(a_{33}-\lambda - \cfrac{a_{32}a_{23}}{a_{22}-\lambda-\ldots} - \ldots\right)\left(a_{22}-\lambda - \cfrac{a_{24}a_{42}}{a_{44}-\lambda-\ldots} - \ldots\right)} \end{aligned} \tag{33}$$

which may be solved iteratively for the λ's. Thus the first approximation gives

$$\lambda = a_{11} - \cfrac{a_{12}a_{21}}{a_{22}-a_{11}} - \cfrac{a_{13}a_{31}}{a_{33}-a_{11}} - \ldots \tag{34}$$

which may be used as a trial solution in obtaining the second approximation, and so on.

In the case of degeneracy (say $a_{22} = a_{11}$), instead of (34) it is necessary to take the first approximation to x_1 to be given by one of the roots of the quadratic

$$a_{11} - \lambda - \frac{a_{12}a_{21}}{a_{22} - \lambda} - \frac{a_{13}a_{31}}{a_{33} - a_{11}} - \ldots = 0 \tag{35}$$

and similarly for the higher iterations. The idea is to treat the roots near $\lambda = a_{11}$ and $\lambda = a_{22}$ as being of equal importance.

An example of a situation where eigenvalues have been found numerically and analytically by such methods is provided by Swain (1974), and analytically by McClean and Swain (1976).

We conclude by briefly discussing some of the numerical aspects of this method of finding eigenvalues. It is an iterative method of the form

$$\lambda_i^{(n)} = f(\lambda_i^{(n-1)}) \tag{36}$$

and so the usual condition for convergence of the iterative approach, namely

$$|f'(\lambda_i)| < 1 \tag{37}$$

applies, where λ_i is the exact value of the desired root. Thus if a first approximation to λ_i can be found, the present method may be used to find *all* the eigenvalues for which condition (37) holds. In the conventional iterative methods, it is usually much simpler to find the largest or the smallest eigenvalue than a general one. Obviously, the smaller the number of terms in the series in expression (33), the simpler the function $f(\lambda)$, and so once again we would expect this method to be particularly rapid for sparse matrices (or equivalently, recurrence relations with relatively few terms). Thus for a tridiagonal matrix, the function $f(\lambda)$ is just a single continued fraction, and the iterative procedure is very simple. This was the case for the system investigated in Swain (1974). For a pentadiagonal matrix, $f(\lambda)$ would be the sum of two terms, the first a simple continued fraction, the second a product of two continued fractions so that the procedure is slightly more complicated.

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