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1977 J. Phys. A: Math. Gen. 10 155

(http://iopscience.iop.org/0305-4470/10/2/004)

J. Phys. A: Math. Gen., Vol. 10, No. 2, 1977. Printed in Great Britain. © 1977

Continued fraction solutions in degenerate perturbation theory

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Received 23 September 1976

Abstract. A generalization of a previously derived expansion of a determinant in terms of determinants of progressively lower order is obtained and used to discuss the eigenvalue problem in the cases when two or more elements are degenerate. The development is exact for the case of a finite determinant, and represents a perturbation series for an infinite determinant. A procedure is given for writing down the expansion to any order without using detailed algebra. An application to inhomogeneous systems of linear equations is also briefly discussed. The continued fraction methods are more straightforward to apply (particularly for the higher orders) and are more rapidly convergent than standard perturbation theory.

1. Introduction

In a previous publication (Swain 1976, to be referred to as I) we have discussed continued fraction solutions to systems of linear equations which are particularly useful in the absence of degeneracy. To illustrate the main points of interest here we first of all consider the eigenvalue problem

$$\det (a_{ij} - \lambda \delta_{ij}) = 0. \tag{1}$$

In the final section of I we considered an iterative method of obtaining the eigenvalues λ in the situation where the diagonal elements a_{ii} were much larger than the off-diagonal elements, a_{ij} $(i \neq j)$. A zeroth order approximation to the eigenvalue λ_p is then

$$\lambda_p^{(0)} = a_{pp} \tag{2}$$

and an iterative scheme was described for obtaining the higher order approximations. This procedure may run into difficulties when there is *degeneracy*, that is, where there exists another diagonal element, a_{qq} say, which is equal (or nearly equal) to a_{pp}. A method of rearranging the equations to avoid this difficulty was described, and although this would be straightforward to apply in the case of single degeneracy, it would be much more difficult to deal with multiple degeneracy $a_{pp} = a_{qq} = a_{rr} \ldots$. Accordingly, in this paper we develop a general method for dealing with degeneracies of any multiplicity. A simple procedure for writing down an appropriate form of the eigenvalue equation to any desired order is given.

The advantages of the present method over conventional degenerate perturbation theory are: (*a*) for a finite determinant the series terminates and is exact; (*b*) the continued fraction structure usually ensures much more rapid convergence than a power series development; (*c*) extension to higher orders is simple and straightforward; and (*d*) the convergence of the iteration process in any order is not affected by problems of degeneracy. Thus the numerical procedures are much simpler.

In § 2 we obtain an expansion for a determinant in terms of determinants of lower order which is used to develop the continued fraction structure. This is particularly useful when two diagonal elements are equal. A set of rules for writing down the expansion to any order is given; these rules apply with obvious generalizations to the situation where three or more diagonal elements are equal. In § 3 we discuss the eigenvalue problem in detail, and in § 4 we consider higher order degeneracy. Finally, in § 5 we discuss very briefly the problem of inhomogeneous linear equations.

The methods described here are perhaps particularly useful in quantum theory, but the discussion given is quite general.

2. Expansion of a determinant by two elements

In I, the following expansion of the determinant of a matrix, $\mathscr{A} \equiv \det(a_{ij})$, was used to develop the continued fraction theory:

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

where $\mathscr{A}^{\alpha,\beta,\gamma,\dots}$ denotes the determinant obtained from $\mathscr{A}$ by deleting the αth, βth, γth, ... rows and columns. For a finite determinant the series terminates, and the resulting expansion is exact. Note that if $\mathscr{A}$ is a determinant of the Nth order, we must adopt the convention that

$$\mathscr{A}^{1,2,3,\dots,N-1,N} = 1 \tag{4}$$

(i.e. the determinant obtained from $\mathscr{A}$ by deleting all its rows and columns has the value unity). Let us introduce the term *state* for the suffices of a_{ij}. The significant feature of the expansion (3) for our present purposes is that all the determinants on the right-hand side contain no coefficients involving the state j. Suppose two states p and q are degenerate. We wish to obtain an expansion for $\mathscr{A}$ in terms of determinants which do not involve the states p and q. It will be seen later that by doing this no problems associated with the degeneracy of the states p and q will arise. Setting $j = p$ in (3) we see that we have to consider determinants of the type $\mathscr{A}^{p}$, $\mathscr{A}^{\alpha,p}$, $\mathscr{A}^{\alpha,\beta,p}$, ... which may themselves be expanded using (3). We take the leading element in each case to be a_{qq}, when we obtain

$$\mathscr{A}^{p} = a_{qq}\mathscr{A}^{p,q} - \sum_{\alpha\neq p,q} a_{q\alpha}a_{\alpha q}\mathscr{A}^{\alpha,p,q} + \sum_{\alpha\neq p,q}\sum_{\beta\neq\alpha,p,q} a_{q\alpha}a_{\alpha\beta}a_{\beta q}\mathscr{A}^{\alpha,\beta,p,q} + \dots \tag{5}$$

$$\mathscr{A}^{\alpha,p} = a_{qq}\mathscr{A}^{\alpha,p,q} - \sum_{\beta\neq\alpha,p,q} a_{q\beta}a_{\beta q}\mathscr{A}^{\alpha,\beta,p,q} + \sum_{\beta\neq\alpha,p,q}\sum_{\gamma\neq\alpha,\beta,p,q} a_{q\beta}a_{\beta\gamma}a_{\gamma q}\mathscr{A}^{\alpha,\beta,\gamma,p,q}\dots \tag{6}$$

and so on. If we substitute these expressions into (3) we obtain an expansion for $\mathscr{A}$ in terms of determinants in which all reference to the selected states p and q is deleted. Explicitly, we obtain

$$\begin{aligned}\mathscr{A} = (a_{pp}a_{qq} - a_{pq}a_{qp})\mathscr{A}^{p,q} \\ - \sum_{\alpha \neq p,q} (a_{pp}a_{q\alpha}a_{\alpha q} + a_{qq}a_{p\alpha}a_{\alpha p} - a_{pq}a_{q\alpha}a_{\alpha p} - a_{p\alpha}a_{\alpha q}a_{qp})\mathscr{A}^{\alpha,p,q} \\ + \sum_{\alpha \neq p,q} \sum_{\beta \neq \alpha,p,q} (a_{pp}a_{q\alpha}a_{\alpha\beta}a_{\beta q} + a_{qq}a_{p\alpha}a_{\alpha\beta}a_{\beta p} + a_{p\alpha}a_{\alpha p}a_{q\beta}a_{\beta q} \\ - a_{pq}a_{q\alpha}a_{\alpha\beta}a_{\beta p} - a_{p\alpha}a_{\alpha q}a_{q\beta}a_{\beta q} - a_{p\alpha}a_{\alpha\beta}a_{\beta q}a_{qp})\mathscr{A}^{\alpha,\beta,p,q} + \dots \end{aligned} \tag{7}$$

We emphasize that for a finite determinant the expansion terminates and is exact.

To express this in a form suitable for a continued fraction expansion we divide both sides of equation (7) by $\mathscr{A}^{p,q}$:

$$\begin{aligned}\mathscr{A}/\mathscr{A}^{p,q} = a_{pp}a_{qq} - a_{pq}a_{qp} \\ - \sum_{\alpha \neq p,q} (a_{pp}a_{q\alpha}a_{\alpha q} + a_{qq}a_{p\alpha}a_{\alpha p} - a_{pq}a_{q\alpha}a_{\alpha p} - a_{p\alpha}a_{\alpha q}a_{qp})/\mathscr{D}_{\alpha}^{pq} \\ + \sum_{\alpha \neq p,q} \sum_{\beta \neq \alpha,p,q} (a_{pp}a_{q\alpha}a_{\alpha\beta}a_{\beta q} + a_{qq}a_{p\alpha}a_{\alpha\beta}a_{\beta p} + a_{p\alpha}a_{\alpha p}a_{q\beta}a_{\beta q} \\ - a_{pq}a_{q\alpha}a_{\alpha\beta}a_{\beta p} - a_{p\alpha}a_{\alpha q}a_{q\beta}a_{\beta p} - a_{p\alpha}a_{\alpha\beta}a_{\beta q}a_{qp})/\mathscr{D}_{\alpha\beta}^{pq} + \dots \end{aligned} \tag{8}$$

where the $\mathscr{D}$ functions are defined by the relations

$$\mathscr{D}_{\alpha}^{pq} \equiv \frac{\mathscr{A}^{pq}}{\mathscr{A}^{pq\alpha}}, \qquad \mathscr{D}_{\alpha\beta}^{pq} = \frac{\mathscr{A}^{pq}}{\mathscr{A}^{pq\alpha\beta}}, \qquad \text{etc.} \tag{9}$$

We note that the second of the expressions (9) may be written

$$\mathscr{D}_{\alpha\beta}^{pq} = \frac{\mathscr{A}^{pq}}{\mathscr{A}^{pq\alpha}} \frac{\mathscr{A}^{pq\alpha}}{\mathscr{A}^{pq\alpha\beta}} = \mathscr{D}_{\alpha}^{pq}\mathscr{D}_{\beta}^{pq\alpha}. \tag{10}$$

Equation (10) is an example of the more general relationship

$$\mathscr{D}_{\alpha\beta\gamma\dots\lambda}^{pq}\mathscr{D}_{\mu}^{pq\alpha\beta\gamma\dots\lambda} = \mathscr{D}_{\alpha\beta\gamma\dots\lambda\mu}^{pq}. \tag{11}$$

According to I, equation (10), we have the following expressions for the $\mathscr{D}_n^{ij\dots lm}$:

$$\mathscr{D}_n^{ij\dots lm} = a_{nn} - \sum_{\alpha \neq i,j\dots mn} \frac{a_{n\alpha}a_{\alpha n}}{\mathscr{D}_{\alpha}^{ij\dots lmn}} + \sum_{\alpha \neq i,j\dots mn} \sum_{\beta \neq i,j\dots mn\alpha} \frac{a_{n\alpha}a_{\alpha\beta}a_{\beta n}}{\mathscr{D}_{\alpha}^{ij\dots mn}\mathscr{D}_{\beta}^{ij\dots mn\alpha}} + \dots \tag{12}$$

Repeated use of expression (12) for the higher order $\mathscr{D}$ functions which appear in the denominators of the right-hand side of this equation produces a continued fraction structure.

Instead of expressing $\mathscr{D}_{\alpha\beta}^{pq}$ as the product of two $\mathscr{D}$ functions with single suffices, we may obtain an expansion for it directly by considering the expression for $\mathscr{A}^{pq}/\mathscr{A}^{pq\alpha\beta}$

expanded according to (8):

$$\begin{aligned}\mathscr{D}^{pq}_{\alpha\beta} &\equiv \mathscr{A}^{pq}/\mathscr{A}^{pq\alpha\beta} \\ &= (a_{\alpha\alpha}a_{\beta\beta} - a_{\alpha\beta}a_{\beta\alpha}) - \sum_{\gamma\neq\alpha\beta pq} (a_{\alpha\alpha}a_{\beta\gamma}a_{\gamma\beta} \\ &\quad + a_{\beta\beta}a_{\alpha\gamma}a_{\gamma\alpha} - a_{\alpha\beta}a_{\beta\gamma}a_{\gamma\alpha} - a_{\alpha\gamma}a_{\gamma\beta}a_{\beta\alpha})/\mathscr{D}^{pq\alpha\beta}_{\gamma} \\ &\quad + \sum_{\gamma\neq\alpha\beta pq}\ \sum_{\delta\neq\alpha\beta\gamma pq} (a_{\alpha\alpha}a_{\beta\gamma}a_{\gamma\delta}a_{\delta\beta} + \ldots)/\mathscr{D}^{pq\alpha\beta}_{\gamma\delta} + \ldots .\end{aligned} \tag{13}$$

Before discussing the implications of equation (8) it is worthwhile examining its structure to see whether we can determine any pattern in the terms which appear. We may divide the combinations of coefficients a_{ij} appearing in equation (8) into two types: reducible (or disconnected) and irreducible (or connected). An irreducible combination is one in which the final state of one coefficient is identical to the initial state of the following coefficient. Thus $a_{pq}a_{q\alpha}a_{\alpha\beta}a_{\beta p}$ is irreducible (connected) and may be represented by the irreducible (connected) process

$$p \to q \to \alpha \to \beta \to p. \tag{14}$$

A reducible combination is one which splits up into the product of two or more irreducible combinations; it may be represented by a reducible (or disconnected) process. Thus the combination $a_{p\alpha}a_{\alpha p}a_{q\beta}a_{\beta q}$ is reducible, and is represented by the process

$$p \to \alpha \to p; \qquad q \to \beta \to q, \tag{15}$$

which is clearly the product of two irreducible processes. Note that in both types of combination, no two initial states and no two final states are identical, but each initial state is identical to one final state. In every irreducible combination in equation (8) the *principle states* p and q both appear, whereas in the reducible combinations p always appears in one factor and q in the other.

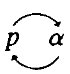
Since we may write

$$a_{p\alpha}a_{\alpha p} = a_{\alpha p}a_{p\alpha} \tag{16}$$

the processes corresponding to this combination may be written in either of the two ways

$$p \to \alpha \to p \qquad \text{or} \qquad \alpha \to p \to \alpha. \tag{17}$$

A logically satisfactory way to represent this term would be as a cyclic process



(18)

but as this is cumbersome, especially for combinations of higher order, we do not adopt this approach. Instead it should be understood that the initial and final states are identical, although this is not shown explicitly:

$$p \to \alpha \to p \equiv \underline{\to p \to \alpha \to p \to}\ . \tag{19}$$

Following the principles listed in the previous two paragraphs we may list all the combinations which contribute to equation (8) as follows:

Order	*Reducible*	*Irreducible*	
Second	$p\to p;\, q\to q$	$p\to q\to p$	
Third	$p\to p;\, q\to\alpha\to q$ $p\to\alpha\to p;\, q\to q$	$p\to q\to\alpha\to p$ $p\to\alpha\to q\to p$	(20)
Fourth	$p\to p;\, q\to\alpha\to\beta\to q$ $p\to\alpha\to p;\, q\to\beta\to q$ $p\to\alpha\to\beta\to p;\, q\to q$	$p\to q\to\alpha\to\beta\to p$ $p\to\alpha\to q\to\beta\to p$ $p\to\alpha\to\beta\to q\to p.$	

The states $\alpha, \beta, \ldots$ which must be different from p or q we will refer to as *intermediate states.* It is easy to see that this list includes all the reducible and irreducible processes involving the principal states p and q up to and including the fourth order.

The contribution of each process to $\mathscr{A}/\mathscr{A}^{pq}$ is obtained by the following procedure: with each transition $i\to j$ associate the factor a_{ij}; take the product of all such coefficients, together with the factor $(-1)^{n+r}/\mathscr{D}^{pq}_{\alpha\beta\ldots\mu}$ where $\alpha, \beta, \ldots, \mu$ is a list of all the intermediate states which appear in the process, n is the order of the process, and r is the number of reducible factors in this process. (In this section r is always equal to 1 or 2). For example, the process

$$p\to p;\, q\to\alpha\to\beta\to q \tag{21}$$

makes the contribution

$$(-1)^{4+2}a_{pp}a_{q\alpha}a_{\alpha\beta}a_{\beta q}/\mathscr{D}^{pq}_{\alpha\beta}. \tag{22}$$

Adding all such contributions up to order n gives the expansion of $\mathscr{A}/\mathscr{A}^{pq}$ to this order.

We thus have a way of obtaining our expression for $\mathscr{A}/\mathscr{A}^{pq}$ to any order without the labour of performing the direct substitutions necessary in first obtaining expression (8): we merely list all the reducible and irreducible processes involving the principal states p and q, and associate contributions with them as previously described.

More succinct expressions may be obtained by employing the notation:

$\langle pq\rangle$ ≡ contribution of reducible and irreducible processes involving the principal states p and q only,

$\langle pq;\alpha\rangle$ ≡ contribution of reducible and irreducible processes involving the principal states, p and q, and the one intermediate state α,

⋮

Then equation (8) may be written

$$\frac{\mathscr{A}}{\mathscr{A}^{pq}}=\langle pq\rangle-\sum_{\alpha\neq pq}\frac{\langle pq;\alpha\rangle}{\mathscr{D}^{pq}_{\alpha}}+\sum_{\alpha\neq pq}\sum_{\beta\neq\alpha pq}\frac{\langle pq;\alpha\beta\rangle}{\mathscr{D}^{pq}_{\alpha\beta}}+\ldots \tag{23}$$

and equation (13) as

$$\mathscr{D}^{pq}_{\alpha\beta}=\langle\alpha\beta\rangle-\sum_{\gamma\neq\alpha\beta pq}\frac{\langle\alpha\beta;\gamma\rangle}{\mathscr{D}^{pq\alpha\beta}_{\gamma}}+\sum_{\gamma\neq\alpha\beta pq}\sum_{\delta\neq\alpha\beta\gamma pq}\frac{\langle\alpha\beta;\gamma\delta\rangle}{\mathscr{D}^{pq\alpha\beta}_{\gamma\delta}}+\ldots. \tag{24}$$

Finally, we rearrange equation (8) into a more compact form. We note that the terms involving the diagonal elements a_{pp} and a_{qq} in equation (8) may be written

$$a_{pp}a_{qq} - a_{pp}\left(\sum_{\alpha\neq pq}\frac{a_{q\alpha}a_{\alpha q}}{\mathscr{D}^{pq}_{\alpha}} - \sum_{\alpha\neq pq}\sum_{\beta\neq\alpha pq}\frac{a_{q\alpha}a_{\alpha\beta}a_{\beta q}}{\mathscr{D}^{pq}_{\alpha\beta}} + \ldots\right)$$

$$- a_{qq}\left(\sum_{\alpha\neq pq}\frac{a_{p\alpha}a_{\alpha p}}{\mathscr{D}^{pq}_{\alpha}} - \sum_{\alpha\neq pq}\sum_{\beta\neq\alpha pq}\frac{a_{p\alpha}a_{\alpha\beta}a_{\beta p}}{\mathscr{D}^{pq}_{\alpha\beta}} + \ldots\right)$$

$$= a_{pp}a_{qq} - a_{pp}W^{p}_{q} - a_{qq}W^{q}_{p} \tag{25}$$

$$= (a_{pp} - W^{q}_{p})(a_{qq} - W^{p}_{q}) - W^{p}_{q}W^{q}_{p} \tag{26}$$

where

$$W^{p}_{q} = \sum_{\alpha\neq pq}\frac{a_{q\alpha}a_{\alpha q}}{\mathscr{D}^{pq}_{\alpha}} - \sum_{\alpha\neq pq}\sum_{\beta\neq\alpha pq}\frac{a_{q\alpha}a_{\alpha\beta}a_{\beta q}}{\mathscr{D}^{pq}_{\alpha\beta}} + \ldots \tag{27}$$

is equivalent to the sum of all irreducible contributions from q to q with the state p excluded.

By comparing expression (27) and (12) it is clear that

$$W^{p}_{q} = \mathscr{D}^{p}_{q} - a_{qq}. \tag{28}$$

Hence we may write equation (8) as

$$\mathscr{A}/\mathscr{A}^{pq} = \mathscr{D}^{p}_{q}\mathscr{D}^{q}_{p} - W^{p}_{q}W^{q}_{p} - U_{pq} \tag{29a}$$

$$= (a_{pp} - W^{q}_{p})(a_{qq} - W^{p}_{q}) - W^{p}_{q}W^{q}_{p} - U_{pq} \tag{29b}$$

where $(-U_{pq})$ is the contribution of the off-diagonal terms in equation (8), i.e.

$$U_{pq} = a_{pq}a_{qp} - \sum_{\alpha\neq pq}(a_{pq}a_{q\alpha}a_{\alpha p} + a_{p\alpha}a_{\alpha q}a_{qp})/\mathscr{D}^{pq}_{\alpha}$$

$$+ \sum_{\alpha\neq pq}\sum_{\beta\neq\alpha pq}(a_{pq}a_{q\alpha}a_{\alpha\beta}a_{\beta q} + a_{p\alpha}a_{\alpha q}a_{q\beta}a_{\beta p}$$

$$+ a_{p\alpha}a_{\alpha\beta}a_{\beta q}a_{qp} - a_{p\alpha}a_{\alpha p}a_{q\beta}a_{\beta q})/\mathscr{D}^{pq}_{\alpha\beta} + \ldots. \tag{30}$$

We now consider the eigenvalue problem (1). The determinant in that equation is obtained from $\mathscr{A}$ by replacing every diagonal element a_{ii} by $(a_{ii} - \lambda)$. Consequently, using this prescription and equation (29*b*), the eigenvalue problem (1) becomes equivalent to

$$(a_{pp} - \lambda - W^{q}_{p}(\lambda))(a_{qq} - \lambda - W^{p}_{q}(\lambda)) = W^{p}_{q}(\lambda)W^{q}_{p}(\lambda) + U_{pq}(\lambda) \tag{31}$$

where we have indicated explicitly that the W's and U are now functions of λ.

3. The eigenvalue problem

Before considering the application of equation (31) to the degenerate eigenvalue problem we illustrate the problems that can arise in applying the methods described in I in these circumstances. As an example, we consider the problem of finding the eigenvalues of the Hermitian matrix

$$\begin{bmatrix} E_1 & V_{12} & V_{13} & V_{14} & \dots \\ V_{12} & E_2 & V_{23} & V_{26} & \dots \\ V_{13} & V_{23} & E_3 & V_{34} & \dots \\ \vdots & \vdots & \vdots & \vdots & \end{bmatrix} \tag{32}$$

where $|V_{ij}|^2 \ll E_i$ for all i and j. According to equation (32) of I the first few terms in the eigenvalue equation for this matrix may be written (supposing we want the eigenvalue near E_1)

$$E_1 - \lambda - \cfrac{|V_{12}|^2}{E_2 - \lambda - \cfrac{|V_{23}|^2}{E_3 - \lambda - \dots}} - \cfrac{|V_{13}|^2}{E_3 - \lambda - \cfrac{|V_{23}|^2}{E_2 - \lambda - \dots}} - \dots = 0. \tag{33}$$

To solve equation (33) iteratively we might take $\lambda^{(0)} = E_1$ as the zeroth order approximation. A first iteration then gives

$$\lambda^{(1)} = E_1 - \sum_{\alpha \neq 1} \frac{|V_{\alpha 1}|^2}{E_\alpha - E_1} \tag{34}$$

which is satisfactory unless there is degeneracy (or near degeneracy). Suppose for example $E_2 = E_1$: then if $|V_{12}| \neq 0$ the expression (34) diverges. In this case one can get around the problem by solving for the roots near $\lambda = E_1$ and $\lambda = E_2$ simultaneously, as described in I (cf equation (34) of I). However, even if $|V_{12}| = 0$, although (34) is then apparently satisfactory as a first iteration, we do not avoid the difficulty—it merely reappears in the higher iterations. Thus in the second iteration, the denominator in the final term of (33) contains the term $-|V_{23}|^2/(E_2 - \lambda)$ which on substituting for λ from (34), is of the order of unity in the degenerate case, whereas in the non-degenerate case it is of the order of $|V_{23}|^2/(E_2 - E_1)$. Clearly the convergence of the iteration scheme will be disrupted.

Let us now use equation (31) with $p = 1, q = 2$ to tackle the degenerate problem. No difficulties of the type encountered in equation (33) will occur here, as the $\mathscr{D}$ functions which appear in equation (31) are all of the type $\mathscr{D}_\alpha^{1,2}$, $\mathscr{D}_{\alpha,\beta}^{1,2}$, etc, which means that the terms $(\lambda - E_1)$, $(\lambda - E_2)$ *never appear in the denominators*. Retaining only contributions up to and including fourth order in the $|V_{ij}|$ and collecting together a few terms on the right-hand side, we obtain (setting $E_1 = E_2 = \bar{E}$),

$$\begin{aligned} &\left(\lambda - \bar{E} + \sum_{\alpha \neq 1,2} \frac{|V_{\alpha 1}|^2}{\bar{E} - E_\alpha}\right)\left(\lambda - \bar{E} + \sum_{\alpha \neq 1,2} \frac{|V_{\alpha 2}|^2}{\bar{E} - E_\alpha}\right) \\ &\quad = \left(\sum_{\alpha \neq 1,2} \frac{V_{1\alpha} V_{\alpha 2}}{\bar{E} - E_\alpha}\right)\left(\sum_{\beta \neq 1,2} \frac{V_{2\beta} V_{\beta 1}}{\bar{E} - E_\beta}\right) + \left(|V_{12}|^2 - \sum_{\alpha \neq 1,2} \frac{V_{12} V_{2\alpha} V_{\alpha 1} + V_{1\alpha} V_{\alpha 2} V_{21}}{\lambda^{(1)} - E_\alpha}\right. \\ &\qquad \left. + \sum_{\alpha \neq 1,2} \sum_{\beta \neq \alpha,1,2} \frac{V_{12} V_{2\alpha} V_{\alpha\beta} V_{\beta 1} + V_{1\alpha} V_{\alpha\beta} V_{\beta 2} V_{21}}{(\bar{E} - E_\alpha)(\bar{E} - E_\beta)}\right). \end{aligned} \tag{35}$$

We have taken the zeroth order approximation to the $\mathscr{D}$ functions in equation (32), e.g.

$$\mathscr{D}_\alpha^{1,2}(\lambda) \simeq \lambda - E_\alpha + \mathrm{O}(|V_{ij}|^2) \simeq \bar{E} - E_\alpha + \mathrm{O}(|V_{ij}|) \tag{36}$$

except for the term which corresponds to the second one in the final large parentheses of equation (35), where, to be consistent to fourth order, we should replace λ not by $\bar{E}$, but by its value correct to first order in $|V_{ij}|$, $\lambda^{(1)}$.

We first consider the case where $|V_{12}| \neq 0$. Clearly the lowest non-trivial approximation is

$$(\lambda - \bar{E})(\lambda - \bar{E}) = |V_{12}|^2 \tag{37}$$

which gives the first-order solution

$$\lambda_{\pm}^{(1)} = \bar{E} \pm |V_{12}|. \tag{38}$$

To obtain the second approximation we may omit the first and last terms on the right-hand side of equation (35), and also set $\lambda^{(1)} = \bar{E}$. This gives

$$\lambda_{\pm}^{(2)} = \bar{E} - \tfrac{1}{2} \sum_{\alpha \neq 1,2} \frac{|V_{\alpha 1}|^2 + |V_{\alpha 2}|^2}{\bar{E} - E_\alpha} \pm \left(|V_{12}|^2 - \sum_{\alpha \neq 1,2} \frac{V_{12} V_{2\alpha} V_{\alpha 1} + V_{1\alpha} V_{\alpha 2} V_{21}}{\bar{E} - E_\alpha} \right)^{1/2} \tag{39}$$

or, on expanding the square root,

$$\lambda_{\pm}^{(2)} \doteqdot \bar{E} \pm |V_{12}| - \tfrac{1}{2} \sum_{\alpha \neq 1,2} \frac{|V_{\alpha 1}\, e^{-\frac{1}{2}i\phi} \pm V_{\alpha 2}\, e^{-\frac{1}{2}i\phi}|^2}{\bar{E} - E_\alpha} \tag{40}$$

where $V_{12} \equiv |V_{12}|\, e^{i\phi}$. Expression (40) is identical with the standard expressions obtained by other means (cf equation (175) of A Dalgarno in Bates 1961). The formulae for the higher orders rapidly become very complicated (cf equation (176) of Dalgarno). The advantage of the present method is that, when applied to a definite problem where the E_i and V_{ij} are known numerically, it is straightforward to write down equation (31) to any desired degree of accuracy, and it may then be solved iteratively in the manner indicated through equations (37) to (40).

The case where $|V_{12}| = 0$ is easily dealt with; in this event the last bracketed expression on the right-hand side of equation (35) vanishes, and one is left with a quadratic equation to solve for the λ's, which is identical to that which would be obtained from the standard methods of perturbation theory (see e.g. Schiff 1955 equation (25.24)).

4. Expansion of a determinant by three or more elements

We may extend the procedure of § 2 to obtain an expansion of the determinant $\mathscr{A}$ in terms of determinants of lower order which contain no reference to the states p, q, r, s, ... Consider first the case where three states p, q and r are to be excluded. Starting from equation (7), we could substitute the expansions

$$\mathscr{A}^{pq} = a_{rr} \mathscr{A}^{p,q,r} - \sum_{\alpha \neq pqr} a_{r\alpha} a_{\alpha r} \mathscr{A}^{\alpha pqr} + \dots \tag{41}$$

$$\mathscr{A}^{\alpha pq} = a_{rr} \mathscr{A}^{\alpha pqr} - \sum_{\beta \neq \alpha pqr} a_{r\beta} a_{\beta r} \mathscr{A}^{\alpha\beta pqr} + \dots \tag{42}$$

etc, in the right-hand side, and simplify. However, it turns out that we can obtain the same result by listing all the reducible and irreducible processes involving the three principal states p, q and r, and associating contributions (with obvious generalizations) with them as described in § 2. The lowest order processes are third order, and these and the fourth order processes are listed below:

Third order

$p\to p; q\to q; r\to r$	$p\to p; q\to r\to q$
$q\to q; p\to r\to p$	$r\to r; p\to q\to p$
$p\to q\to r\to p$	$p\to r\to q\to p$

Fourth order

$p\to p; q\to q; r\to \alpha\to r$	$p\to p; q\to \alpha\to q; r\to r$
$p\to p; q\to \alpha\to r\to p$	$p\to p; q\to r\to \alpha\to p$
$q\to q; r\to r; p\to \alpha\to p$	$q\to q; p\to \alpha\to r\to p$
$q\to q; p\to r\to \alpha\to p$	$r\to r; p\to \alpha\to q\to p$
$r\to r; p\to q\to \alpha\to p$	$p\to q\to p; r\to \alpha\to r$
$p\to \alpha\to p; q\to r\to q$	$p\to r\to p; q\to \alpha\to q$
$p\to q\to \alpha\to r\to p$	$p\to \alpha\to r\to q\to p$
$p\to \alpha\to q\to r\to p$	$p\to q\to r\to \alpha\to p$
$p\to r\to q\to \alpha\to p$	$p\to r\to \alpha\to q\to p.$

(43)

Writing down the contributions of these processes as described in § 2 we obtain

$$\begin{aligned}\frac{\mathscr{A}}{\mathscr{A}^{pqr}} &= \langle pqr\rangle - \sum_{\alpha\neq pqr}\frac{\langle pqr;\alpha\rangle}{\mathscr{D}_\alpha^{pqr}} + \ldots \\ &= a_{pp}a_{qq}a_{rr} - a_{pp}a_{qr}a_{rq} - a_{qq}a_{pr}a_{rp} - a_{rr}a_{pq}a_{qp} + a_{pq}a_{qr}a_{rp} + a_{pr}a_{rq}a_{qp} \\ &\quad + \sum_{\alpha\neq pqr}(-a_{pp}a_{qq}a_{r\alpha}a_{\alpha r} - a_{pp}a_{rr}a_{q\alpha}a_{\alpha q} + a_{pp}a_{q\alpha}a_{\alpha r}a_{rp} + a_{pp}a_{qr}a_{r\alpha}a_{\alpha p} \\ &\quad - a_{qq}a_{rr}a_{p\alpha}a_{\alpha p} + a_{qq}a_{p\alpha}a_{\alpha r}a_{rp} + a_{qq}a_{pr}a_{r\alpha}a_{\alpha p} + a_{rr}a_{p\alpha}a_{\alpha q}a_{qp} + a_{rr}a_{pq}a_{q\alpha}a_{\alpha p} \\ &\quad + a_{pq}a_{qp}a_{r\alpha}a_{\alpha r} + a_{p\alpha}a_{\alpha p}a_{qr}a_{rq} + a_{pr}a_{rp}a_{q\alpha}a_{\alpha q} - a_{pq}a_{q\alpha}a_{\alpha r}a_{rp} - a_{p\alpha}a_{\alpha r}a_{rq}a_{qp} \\ &\quad - a_{p\alpha}a_{\alpha q}a_{qr}a_{rp} - a_{pq}a_{qr}a_{r\alpha}a_{\alpha p} - a_{pr}a_{rq}a_{q\alpha}a_{\alpha p} - a_{pr}a_{r\alpha}a_{\alpha q}a_{qp})/\mathscr{D}_\alpha^{pqr} + \ldots.\end{aligned} \tag{44}$$

This expansion is clearly quite complicated but it must be remembered that in many applications some of the a_{ij} will be zero. Thus if we have

$$a_{pq} = a_{qr} = a_{rp} = 0 \tag{45}$$

the above expression simplifies to

$$\frac{\mathscr{A}}{\mathscr{A}^{pq}} = a_{pp}a_{qq}a_{rr} - \sum_{\alpha\neq pqr}(a_{pp}a_{qq}a_{r\alpha}a_{\alpha r} + a_{pp}a_{rr}a_{q\alpha}a_{\alpha q} + a_{qq}a_{rr}a_{p\alpha}a_{\alpha p})/\mathscr{D}_\alpha^{pqr} + \ldots \tag{46}$$

and the corresponding eigenvalue equation in the degenerate case ($a_{pp} = a_{qq} = a_{rr} = \bar{a}$) becomes

$$(\bar{a}-\lambda)^3 - (\bar{a}-\lambda)^2\sum_{\alpha\neq pqr}\frac{a_{r\alpha}a_{\alpha r} + a_{q\alpha}a_{\alpha q} + a_{p\alpha}a_{\alpha p}}{\bar{a}-\lambda-\ldots} + \ldots = 0. \tag{47}$$

As before, this can be solved by iterative methods. An application of the expansion (44) to a problem involving multi-quantum resonances in a spin-1 atom will be discussed in a forthcoming publication (Hermann and Swain 1976).

5. Inhomogeneous equations

In this section we briefly consider the solution of the (possibly infinite) set of linear, inhomogeneous equations

$$\sum_{\alpha} a_{i\alpha} x_{\alpha} = b_i \tag{48}$$

which as we have shown in I, have the solution

$$x_j = \frac{b_j}{\mathscr{D}_j} - \sum_{\alpha \neq j} \frac{a_{j\alpha} b_{\alpha}}{\mathscr{D}_{\alpha j}} + \sum_{\alpha \neq j} \sum_{\beta \neq \alpha j} \frac{a_{j\beta} a_{\beta\alpha} b_{\alpha}}{\mathscr{D}_{\alpha\beta j}} + \dots . \tag{49}$$

We have discussed the application of solutions of this type to problems in time-dependent quantum mechanical perturbation theory in Swain (1975, to be referred to as II). In this paper the x_j were the Laplace transforms of the time development operator, so that the determinant $\mathscr{A}$ was in fact a function of the Laplace variable $\lambda : \mathscr{A} \equiv \mathscr{A}(\lambda)$. If the inverse Laplace transform is found by the calculus of residues, then, to find the poles, one has to solve

$$\mathscr{A}(\lambda) = 0 \tag{50}$$

—in other words, the eigenvalue problem reappears in a different guise, and with it the problems of degeneracy. We therefore consider the problem of writing equation (49) in a form more suitable for dealing with the degenerate case. For brevity, we consider just the case of two degenerate states, p and q.

By making use of the definition (9) we obtain, for $j \neq p, q$,

$$\frac{1}{\mathscr{D}_j} = \frac{1}{\mathscr{D}_{pq}} \frac{\mathscr{D}^{j}_{pq}}{\mathscr{D}^{pq}_{j}} \tag{51}$$

$$\frac{1}{\mathscr{D}_{\alpha j}} = \frac{1}{\mathscr{D}_{pq}} \frac{\mathscr{D}^{\alpha j}_{pq}}{\mathscr{D}^{pq}_{\alpha j}} \tag{52}$$

and so on. Substituting these expressions into equation (49) we obtain

$$x_j = \frac{1}{\mathscr{D}_{pq}} \left(\frac{b_j \mathscr{D}^{j}_{pq}}{\mathscr{D}^{pq}_{j}} - \sum_{\alpha \neq j} \frac{a_{j\alpha} b_{\alpha} \mathscr{D}^{\alpha j}_{pq}}{\mathscr{D}^{pq}_{\alpha j}} + \sum_{\alpha \neq j} \sum_{\beta \neq \alpha j} \frac{a_{j\beta} a_{\beta\alpha} b_{\alpha} \mathscr{D}^{\alpha\beta j}_{pq}}{\mathscr{D}^{pq}_{\alpha\beta j}} + \dots \right); \qquad j \neq p, q. \tag{53}$$

This is an equation of the desired form, as all the difficulties associated with the degeneracy of the states p and q appear in the factor $1/\mathscr{D}_{pq}(\lambda)$ which is outside the bracket in (53). This factor can be dealt with as described in §§ 2 and 3.

For the case when $j = p$ or q—say $j = p$ to be definite—we have

$$x_p = \frac{1}{\mathscr{D}_{pq}} \left(b_p \mathscr{D}^{p}_{q} - \sum_{\alpha \neq p} \frac{a_{p\alpha} b_{\alpha}}{\mathscr{D}^{pq}_{\alpha}} \mathscr{D}^{\alpha p}_{q} + \sum_{\alpha \neq p} \sum_{\beta \neq \alpha p} \frac{a_{p\beta} a_{\beta\alpha} b_{\alpha} \mathscr{D}^{\alpha\beta p}_{q}}{\mathscr{D}^{pq}_{\alpha\beta}} + \dots \right). \tag{54}$$

To give a trivial illustration of the method, we apply the time-dependent perturbation theory of II to the problem of a two-level atom interacting with a quantized rotating field in the dipole approximation. The Hamiltonian is

$$\mathcal{H} = E_\alpha|\alpha\rangle\langle\alpha| + E_\beta|\beta\rangle\langle\beta| + \hbar\omega a^\dagger a + g(a|\alpha\rangle\langle\beta| + |\beta\rangle\langle\alpha|) \tag{55}$$

where E_α and E_β are the energies of the atom, whose states are $|\alpha\rangle$ and $|\beta\rangle$ respectively, a and $a^\dagger$ are the Bose annihilation and creation operators for a photon of frequency ω, and g is a coupling constant (assumed real for simplicity). We consider the unperturbed states $|p\rangle \equiv |\alpha, n\rangle$, $|q\rangle \equiv |\beta, n+1\rangle$ whose energies are $E_\alpha + n\hbar\omega$, $E_\beta + (n+1)\hbar\omega$ respectively. According to II and equation (54) the Laplace transform of the time-development operator matrix element $U_{pp}(t)$ is given exactly by the relation

$$L_{pp}(z) = \frac{1}{\mathcal{D}_{pq}(z)}(b_p\mathcal{D}_q^p(z) - gb_q) \tag{56}$$

where z is the Laplace variable, and b_p and b_q are the initial weightings of the states p and q. From equations (13) and (12) we readily obtain the exact results

$$\mathcal{D}_{pq}(z) = (E_p - z)(E_q - z) - g^2 \tag{57}$$

and

$$\mathcal{D}_q^p(z) = E_q - z. \tag{58}$$

Hence

$$L_{pp}(z) = \frac{b_p(E_q - z) - gb_q}{(E_p - z)(E_q - z) - g^2}. \tag{59}$$

For simplicity we assume $E_p = E_q = E$, then (59) has poles at $z = E \pm g$, and the inverse Laplace transform gives

$$U_{pp}(t) = -b_p \cos(gt) + ib_q \sin(gt) \tag{60}$$

or, for the probability $P_{pp}(t) = |U_{pp}(t)|^2$,

$$P_{pp}(t) = |b_p|^2 \cos^2(gt) + |b_q|^2 \sin^2(gt). \tag{61}$$

For more complicated systems one would not find finite exact expressions corresponding to equations (56), (57) and (58); instead one would have infinite series and continued fractions which would have to be approximated by truncation at an appropriate stage.

Acknowledgment

The research reported was accomplished with the support of the US Office of Naval Research under Contract N00014-69-C-0035.

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