

ABSTRACT

NONLINEAR PERTURBATIONS OF SPECIAL-FUNCTION OPERATORS

By

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A systematic perturbation theory is presented for the analysis of nonlinear forms of boundary-value problems. In particular, those equations are considered whose unperturbed form belongs to the class of linear special-function equations. The nonlinear terms are then regarded as perturbations of the special-function operators. A matrix representation is obtained for the perturbed operator utilizing the coordinate (Schrödinger) representation of quantum mechanics, truncation and diagonalization of which will determine the perturbed eigenvalues and eigenvectors. In most cases the method is applicable even when the perturbation term is of the same order of magnitude as the remaining terms, or perhaps even larger. To illustrate this point the nonlinear Legendre-like equation $(d/dx)(1 - x^2)(du/dx) + \lambda u + \alpha x^2 u^2 = 0$ is solved for those cases when $\alpha = 1$ and $\alpha = 5$. Other examples include the Hartree equations for the helium atom where a qualitative comparison of the ground state energy is made with experimental data, and a detailed analysis of the van der Pol equation for $\alpha = 0.5$ and $\alpha = 1$.

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1. INTRODUCTION

From the theory of representations it is known that a linear operator L that transforms a Hilbert space into itself gives rise to a matrix representation of that operator.¹ The matrix elements can be defined by the inner product,

$$L_{jk} = (\phi_j, L \phi_k), \quad (1.1)$$

where $\{\phi_k\}$ represents a complete set of orthonormal vectors over the space.

We shall extend such representations to certain nonlinear forms of special-function operators, the matrix elements of which can be computed by algebraic manipulations instead of utilizing expressions like (1.1). The type of nonlinear operator to be considered is represented by the hypergeometric-like form

$$S = \frac{d}{dx} (1 - x^2) \frac{d}{dx} - 2(\mu + \nu x) \frac{d}{dx} + \alpha x^2 u_k, \quad (1.2)$$

from which we obtain the nonlinear eigenequation

$$(S + \lambda_k) u_k = 0. \quad (1.3)$$

The term $\alpha x^2 u_k$ is regarded as a perturbation of the linear hypergeometric operator

$$L = \frac{d}{dx} (1 - x^2) \frac{d}{dx} - 2(\mu + \nu x) \frac{d}{dx}. \quad (1.4)$$

Thus α will serve as the perturbation parameter, but will be treated as a positive constant of arbitrary magnitude in contrast to the usual

restriction that α remain small.² The operator S can now be written

$$S = L + N, \quad (1.5)$$

where $N = \alpha x^2 u_k$. Note that we can further represent N as the product of a linear perturbation αx^2 with a nonlinear perturbation u_k . For $\alpha = 0$, Equation (1.3) becomes a hypergeometric equation with known eigenvalues and eigenvectors.³ We shall seek an eigenvalue-eigenvector solution for Equation (1.3) with $\alpha \neq 0$ that will reduce to the unperturbed solution when we again let $\alpha = 0$.

The perturbation method is of fundamental importance in quantum theory. The mathematical description of noninteracting particles is governed by the (nonrelativistic) Schrödinger equation or by the (relativistic) Klein-Gordon equation.⁴ The separation of variables technique applied to these equations often leads to extended forms of special-function equations. Because direct solution of these equations is usually not possible, approximation methods such as perturbation techniques have proved to be most valuable. In general, though, any basic field equation of the elementary particles cannot be linear since it must define interactions between the particles. Heisenberg suggests that the mathematical form of such an equation should be given by

$$i \sigma^\nu \frac{\partial \chi}{\partial x^\nu} + \ell^2 \sigma^\nu : \chi (\chi^* \sigma_\nu \chi) : = 0, \quad (1.6)$$

where $\chi(x)$ is a local field operator, the σ^ν are the conventional Pauli matrices, and ℓ is an arbitrary constant with the dimension of a length.⁵ (The dots $::$ in the second term refer to the definition

of a product of three field operators at the same space-time point.) The anharmonic oscillator defined by the equation of motion $\ddot{Q} + \alpha Q^3 = 0$, where each dot designates a time derivative, is a simplified representative of (1.6). When equations such as that for the anharmonic oscillator define a conservative holonomic system with time-independent constraints which possesses a kinetic energy that is homogeneous-quadratic, then the system may equally well be described by a linear Schrödinger equation through an application of the Hamilton equations of motion. De Broglie has also suggested the existence of a nonlinear wave equation like (1.6) in accordance with his double solution theory.⁶

Thus it seems natural to consider perturbation methods for approximating solutions of these nonlinear equations. However, the nonlinear terms are ordinarily of the same order of magnitude as the linear terms, so that conventional perturbation theory is not appropriate. It is for this reason, and because of the possible area of application cited, that we present our perturbation method from a quantum mechanical point of view, although this is not essential.

It is most convenient to write differential operators in terms of dynamical variables (observables such as position, momentum, and energy), but these variables must be treated as operators which are generally noncommutative.⁷ The commutations of such operators are proportional to the classical Poisson brackets, i.e.,

$$[Q, R] = QR - RQ = i\{Q, R\} , \quad (1.7)$$

where Q and R represent two quantum mechanical operators and $\{ , \}$ denotes the Poisson brackets.⁸

We wish to write the differential equation (1.3) entirely in terms of dynamic variables. This involves the transformation of the functions $u_k(x)$ of the differential equation to the vectors $\psi^{(k)}(q)$ of the operator equation. Such a transformation can be represented by⁹

$$u_k(x) = \bar{\psi}^{(0)} e^{ipx} \psi^{(k)}(q), \quad (1.8)$$

where x is treated as an unrestricted coordinate variable and where p and q satisfy $qp - pq = i$ (with $\hbar = 1$). In addition to (1.8) we shall also find it useful to establish the two relations

$$x u_k(x) = \bar{\psi}^{(0)} e^{ipx} q \psi^{(k)}, \quad (1.9)$$

$$- i \frac{d}{dx} u_k(x) = \bar{\psi}^{(0)} e^{ipx} p \psi^{(k)}. \quad (1.10)$$

To verify (1.9) we first note that since

$$x e^{ipx} = e^{ipx} q - q e^{ipx}, \quad (1.11)$$

it follows that

$$\begin{aligned} x u_k(x) &= \bar{\psi}^{(0)} x e^{ipx} \psi^{(k)} \\ &= \bar{\psi}^{(0)} e^{ipx} q \psi^{(k)}, \end{aligned} \quad (1.12)$$

where it is assumed that $q \psi^{(0)} = 0$. We verify (1.10) merely by differentiating (1.8). Thus, using (1.8), (1.9), and (1.10) it is easily deduced that

$$\frac{d}{dx} (1 - x^2) \frac{du_k}{dx} = - \bar{\psi}^{(0)} e^{ipx} p(1 - q^2)p \psi^{(k)}, \quad (1.13)$$

$$2(\mu + \nu x) \frac{du_k}{dx} = \bar{\psi}^{(0)} e^{ipx} 2i(\mu + \nu q)p \psi^{(k)}, \quad (1.14)$$

$$\lambda_k u_k = \bar{\psi}^{(0)} e^{ipx} \lambda^{(k)} \psi^{(k)}. \quad (1.15)$$

The nonlinear term in (1.3) requires further analysis in its transformation to operational form. We write

$$\begin{aligned} \alpha x^2 u_k^2 &= \alpha x^2 \bar{\psi}^{(0)} e^{ipx} \psi^{(k)} \bar{\psi}^{(0)} e^{ipx} \psi^{(k)} \\ &= \bar{\psi}^{(0)} e^{ipx} \alpha q^2 \bar{W}(q, \psi^{(k)}) \psi^{(k)} \end{aligned} \quad (1.16)$$

where $\bar{W}(q, \psi^{(k)}) = \psi^{(k)} \bar{\psi}^{(0)} e^{ipx}$ is in general some operator function of q and $\psi^{(k)}$. For most of the applications we have in mind, however, we can express this operator as $\bar{V}(q) \psi^{(k)}$ where, as will be shown in Section 2, $\bar{V}(q)$ is automatically absorbed in the process of forming the matrix elements of the nonlinear operator. Hence, (1.16) becomes

$$\alpha x^2 u_k^2 = \bar{\psi}^{(0)} e^{ipx} \alpha q^2 \bar{V}(q) \psi^{(k)^2}; \quad (1.17)$$

and combining our results we may now rewrite (1.3) in the operational form

$$(A - \lambda^{(k)}) \psi^{(k)} = 0, \quad (1.18)$$

where

$$A = p(1 - q^2)p + 2i(\mu + \nu q)p - \alpha q^2 \bar{V}(q) \psi^{(k)}. \quad (1.19)$$

In general, the operator A may be taken to have the form

$$A = \Gamma(p, q)B(p, q) + \Delta(p, q)Z(p, q, \psi^{(k)}), \quad (1.20)$$

where B represents an unperturbed self-adjoint linear operator, Γ

and Δ represent non-singular linear perturbations, and Z is a non-linear perturbation. For the above case

$$\begin{aligned} B &= p(1 - q^2)p + 2i(\mu + \nu q)p, \\ \Gamma &= 1, \\ \Delta &= -\alpha q^2, \\ Z &= \bar{V}(q) \psi^{(k)}. \end{aligned} \quad (1.21)$$

Two other examples of differential equations with their operational forms are:

$$(1) \quad \frac{d^2 u_k}{dx^2} + (\lambda_k - x^2)u_k + \alpha x^4 u_k^3 = 0,$$

$$[p^2 + q^2 - \alpha q^4 \bar{V}(q) \psi^{(k)^2} - \lambda^{(k)}] \psi^{(k)} = 0,$$

$$B = p^2 + q^2,$$

$$\Gamma = 1,$$

$$\Delta = -\alpha q^4,$$

$$Z = \bar{V}(q) \psi^{(k)^2}.$$

$$(2) \quad (1 - ax^2) \frac{d}{dx} (1 - x^2) \frac{du_k}{dx} + 2\alpha(1 - x^2)xu_k \frac{du_k}{dx} + \lambda_k u_k = 0,$$

$$[(1 - aq^2)p(1 - q^2)p - i\alpha(1 - q^2)qp \bar{V}(q) \psi^{(k)} - \lambda^{(k)}] \psi^{(k)} = 0,$$

$$B = p(1 - q^2)p,$$

$$\Gamma = 1 - aq^2,$$

$$\Delta = -i\alpha(1 - q^2)qp,$$

$$Z = \bar{V}(q) \psi^{(k)}.$$

The unperturbed form ($\alpha = 0$) of Equation (1.18) is given by

$$(B - b^{(k)})U^{(k)} = 0, \quad (1.22)$$

where $b^{(k)}$ and $U^{(k)}$ denote the unperturbed eigenvalues and eigenvectors, respectively. A factorization method for solving linear eigenequations was suggested by Schrödinger, developed in the differential equation form by Infeld and Hull,¹⁰ and given its more recent operational form by Green and Triffet.⁹ The method is also a powerful tool for studying recurrence relations obeyed by the special functions.¹¹

In the factorization method it is generally assumed that for some self-adjoint operator M , whose eigenvalues m we wish to determine, there exist mutually adjoint (adjoint as used here refers to the complex conjugate transpose) linear operators J^+ , J^- , satisfying

$$\begin{aligned} [M, J^+] &= MJ^+ - J^+M \\ &= J^+, \end{aligned} \quad (1.23)$$

$$[M, J^-] = -J^-. \quad (1.24)$$

If, in addition, they satisfy certain other conditions we say the operator B admits a factorization. In particular, if a transformation can be found such that B has the form

$$B = p^2 + w(q), \quad (1.25)$$

then Equation (1.22) can be factorized into the two equations

$$[K(q, M + 1) - ip] U_m^{(j)} = [b^{(j)} - a(m + 1)]^{\frac{1}{2}} U_{m+1}^{(j)} \quad (1.26)$$

$$[K(q, M) + ip] U_m^{(j)} = [b^{(j)} - a(m)]^{\frac{1}{2}} U_{m-1}^{(j)} \quad (1.27)$$

with

$$J^+ = K(q, M + 1) - ip, \quad (1.28)$$

$$J^- = K(q, M) + ip. \quad (1.29)$$

We should point out that Equations (1.26) and (1.27) were originally presented in the differential equation form

$$[K(x, m + 1) - \frac{d}{dx}] u_j^m = [b_j - a(m + 1)]^{\frac{1}{2}} u_j^{m+1}, \quad (1.30)$$

$$[K(x, m) + \frac{d}{dx}] u_j^m = [b_j - a(m)]^{\frac{1}{2}} u_j^{m-1}. \quad (1.31)$$

It has been shown that a necessary and sufficient condition for factorization is that $\underline{K}$ and $\underline{a}$ satisfy the equation

$$\begin{aligned} & \frac{d}{dx} [K(x, m + 1) + K(x, m)] + K^2(x, m + 1) \\ & - K^2(x, m) + a(m + 1) - a(m) = 0. \end{aligned} \quad (1.32)$$

Miller has also shown that Riccati equations similar to (1.32) are sufficient to determine the 4-dimensional Lie algebras $\mathfrak{sl}(a, b)$, whose representations correspond to a study of the special functions of hypergeometric type.¹¹

The factorizations (1.26) and (1.27) now permit us to obtain the eigenvalues and eigenvectors of the operator B in a simple and elegant manner. However, the step operators J^+ , J^- are not unique, as more than one factorization is often possible. In addition, Coulson and Joseph have exploited the use of self-adjoint step

operators.^{12,13}

Green and Triffet have recently introduced a more systematic procedure for determining the step operators.⁹ They have shown that construction of a sequence of linearly independent operators, which do not commute with the unperturbed operator B , will ultimately lead to an appropriate form of the operators. Step operators determined in this fashion will usually not be mutually adjoint. However, they retain their most useful properties and are more general than those defined by the Infeld and Hull factorization technique. Also featured is the basic notational scheme utilized here and an algebraic method for finding matrix representations of linear operators which has been adapted to the present purpose.

2. GENERAL DEVELOPMENT

A. Formulation

A nonlinear differential equation of the form

$$(L + \alpha N + \lambda_k)u_k = 0, \quad (2.1)$$

where L is a linear differential operator, N is a nonlinear differential operator, and α is a constant of arbitrary magnitude, can be treated as a perturbation problem. The boundary conditions will be generally based on physical considerations and referred to as "physical boundary conditions" as opposed to the more common artificially imposed boundary conditions related to the Sturm-Liouville equation.¹⁴ For the special case when $\alpha = 0$ Equation (2.1) becomes linear, so that we shall regard α as the perturbation parameter.

Writing (2.1) in the operational form displaying the quantum mechanical conjugate variables p and q we arrive at

$$(A - \lambda^{(k)})\psi^{(k)} = (\Gamma B + \Delta Z - \lambda^{(k)})\psi^{(k)} = 0; \quad (2.2)$$

thus we make the associations $\Gamma B \rightarrow L$ and $\Delta Z \rightarrow N$. The linear operator L consists of a self-adjoint operator, designated by B , multiplied by a perturbation Γ (ordinarily unity in the examples to be considered). The nonlinear operator N is decomposed so as to separate out the dependency on the eigenvectors $\psi^{(k)}$; consequently, only Z will be a function of $\psi^{(k)}$. Introducing the distinct operators Δ and Z is not necessary but is a convenience for calculating the matrix elements, since Δ may then be interpreted as a linear perturbation.

We seek a matrix representation for A,

$$A_{jk} = \sum_n (\Gamma_{jn} B_{nk} + \Delta_{jn} Z_{nk}), \quad (2.3)$$

diagonalization of which by numerical methods will determine the perturbed eigenvalues. Hence, we find separate matrix representations for each of the operators Γ , B , Δ , and Z . For each choice of a basis which defines our Hilbert space we expect a different, but equivalent, representation. The most convenient basis to select is the set of normalized eigenvectors belonging to the unperturbed operator B ; thus the representation for B is the diagonal matrix

$$B_{jk} = b^{(j)} \delta_{jk}, \quad (2.4)$$

where the $b^{(j)}$ are the eigenvalues of B and $\delta_{jk} = 0$ for $j \neq k$ while $\delta_{jk} = 1$ for $j = k$. We then proceed to determine the matrix representations for Γ , Δ , and Z with respect to this basis.

B. The Operator B

The operator B need be self-adjoint only in the sense that $\bar{B} = \eta B^* \eta^{-1} = B$, where B^* denotes the Hermitian conjugate and η is a positive-definite linear operator. We shall assume that the eigenvalues of B are distinct, nondegenerate and bounded below, but not above, with $b^{(1)}$ as the first eigenvalue. Certain properties are characteristic of such an operator, and these we now list; proofs can be found in the references.^{15,16}

- (1) A linear operator of the second order in p is self-adjoint if and only if it has the form

$$B = pF(q)p + G(q).$$

- (2) For a finite domain the eigenvalues form a denumerably infinite sequence.
- (3) The eigenvalues are real.
- (4) There exists a complete system of associated eigenvectors satisfying the orthonormal relations

$$(\phi^{(j)}, \phi^{(k)}) = \delta_{jk}.$$

We wish to define the step operators $J^{(1)}, J^{(2)}$ associated with B that give the recurrence formulas

$$J^{(1)}U^{(k)} = U^{(k+1)}, \quad (2.5)$$

$$J^{(2)}U^{(k)} = U^{(k-1)}, \quad (2.6)$$

and obey the commutation rule

$$[B, J^{(n)}] = \Lambda^{(n)}J^{(n)}, \quad n = 1, 2 \quad (2.7)$$

where $\Lambda^{(n)}$ designates operators to be determined.

A set of linearly independent operators $J_1, J_2, \dots$, can be considered as a basis for some linear vector space. Hence, any arbitrary operator defined on the space can be represented as a linear combination of the base vectors, and the operators $J^{(n)}$ will have the expansions

$$J^{(n)} = \sum_k J_k \xi_k^{(n)}, \quad n = 1, 2 \quad (2.8)$$

where the $\xi_k^{(n)}$ are components of $J^{(n)}$ in the given basis. Equation (2.8) will define the step operators once the J_k and $\xi_k^{(n)}$ are determined.

Employing (2.8) we note that

$$\begin{aligned} [B, J^{(n)}] &= BJ^{(n)} - J^{(n)}B \\ &= \sum_k (BJ_k - J_k B) \xi_k^{(n)}. \end{aligned} \quad (2.9)$$

Since the J_k form a basis for a linear vector space they must satisfy

$$BJ_k - J_k B = \sum_j J_j c_{jk}, \quad (2.10)$$

where the c_{jk} are either numerical constants or operators which commute with B . This is a consequence of the condition that the operator $[B, J_k]$ must be representable as a linear combination of the base vectors. Substituting (2.10) into (2.9) yields

$$[B, J^{(n)}] = \sum_j \sum_k J_j c_{jk} \xi_k^{(n)}. \quad (2.11)$$

Comparing (2.11) with (2.7) indicates that the operators c_{jk} must comply with the relation

$$\sum_k c_{jk} \xi_k^{(n)} = \Lambda_j^{(n)} \xi_j^{(n)}, \quad (2.12)$$

which identifies $\Lambda_j^{(n)}$ as the eigenvalues of the matrix c_{jk} and $\xi_j^{(n)}$ as the right-eigenvectors. Accordingly, Equation (2.11) becomes

$$\begin{aligned} [B, J^{(n)}] &= \Lambda_j^{(n)} \sum_j J_j \xi_j^{(n)} \\ &= \Lambda_j^{(n)} J^{(n)}. \end{aligned} \quad (2.13)$$

Usually there will only be two nonvanishing eigenvalues $\Lambda^{(n)}$, a positive one designated by $\Lambda^{(1)}$ and a negative one indicated by $\Lambda^{(2)}$.

Equation (2.10) is the defining relation for the sequence of linearly independent operators $J_1, J_2, \dots$. Experience indicates that J_1 should be chosen as an elementary function of the coordinate q and then, forming the commutations

$$\begin{aligned} BJ_1 - J_1 B &= J_1 c_{11} + J_2 c_{21}, \\ BJ_2 - J_2 B &= J_1 c_{12} + J_2 c_{22} + J_3 c_{32}, \\ &\dots \dots \dots \\ BJ_k - J_k B &= \sum_j J_j c_{jk}, \end{aligned} \quad (2.14)$$

successive operators $J_2, \dots$, can be determined. In the examples presented here, where the operator B is a special-function operator, such a sequence will always terminate.

In many cases it is desirable to introduce an operator M , where $B = B(M)$, whose eigenvalues $m^{(k)}$ are separated by unity, i.e., $m^{(k)} = m^{(1)} + k - 1$. Such a device usually simplifies the algebra, as the operator M satisfies the relations

$$MJ^{(1)} = J^{(1)}(M + 1), \quad (2.15)$$

$$MJ^{(2)} = J^{(2)}(M - 1). \quad (2.16)$$

When B is a special-function operator it will be at most a quadratic function in M ,

$$B = a_0 + a_1 M + a_2 M^2, \quad (2.17)$$

where a_1 and a_2 are numerical constants that may be determined from the relations

$$[B, J^{(1)}] = [a_1 + a_2(2M + 1)]J^{(1)}, \quad (2.18)$$

$$[B, J^{(2)}] = -[a_1 + a_2(2M - 1)]J^{(2)}, \quad (2.19)$$

and (2.7). These give

$$\Lambda^{(1)} = a_1 + a_2(2M + 1), \quad (2.20)$$

$$\Lambda^{(2)} = -[a_1 + a_2(2M - 1)], \quad (2.21)$$

which can be solved for a_1 and a_2 . Usually the constant a_0 may be placed equal to zero, but in other cases may be determined from the form of the basic operator B .

Suppose for example $B = p^2 + q^2$. Selecting $J_1 = q$ we have

$$\begin{aligned} [B, J_1] &= p^2q - qp^2 \\ &= -2ip \\ &= 2J_2, \\ [B, J_2] &= -iq^2p + ipq^2 \\ &= 2q \\ &= 2J_1, \end{aligned}$$

where $J_2 = -ip$. The eigenvalues of the matrix c_{jk} are $\Lambda^{(1)} = 2$ and $\Lambda^{(2)} = -2$; the right-eigenvectors are $\underline{\xi}^{(1)} = (1, 1)$ and $\underline{\xi}^{(2)} = (1, -1)$. Thus we obtain the step operators $J^{(1)} = q - ip$ and $J^{(2)} = q + ip$. Substituting $\Lambda^{(1)}$ and $\Lambda^{(2)}$ into Equations (2.20) and (2.21) suggests that $a_1 = 2$ and $a_2 = 0$. Here we have $a_0 = 0$ so that $B = 2M$.

Having the desired step operators $J^{(1)}$ and $J^{(2)}$, we next apply them to the calculation of the eigenvalues and eigenvectors of B . If $U^{(1)}$ denotes the first eigenvector of B then multiplying by $J^{(2)}$ must give

$$J^{(2)}U^{(1)} = 0, \quad (2.22)$$

which follows from Equation (2.6). Multiplying by $J^{(1)}$ yields

$$J^{(1)}J^{(2)}U^{(1)} = 0. \quad (2.23)$$

The operator $J^{(1)}J^{(2)}$ is expressible as a function of B (or M),

$$J^{(1)}J^{(2)} = f(B). \quad (2.24)$$

Therefore the first eigenvalue of B or M is determined from (2.23), which gives

$$f(b^{(1)}) = 0. \quad (2.25)$$

Successive eigenvalues of B can be determined from the relations $m^{(k)} = m^{(1)} + k - 1$ and $B = B(M)$.

To illustrate the above for the operator $B = p^2 + q^2$ we observe that

$$\begin{aligned} f(B) &= J^{(1)}J^{(2)} \\ &= q^2 + iqp - ipq + p^2 \\ &= B - 1 \\ &= 2M - 1. \end{aligned} \quad (2.26)$$

Hence, $m^{(1)} = 1/2$ with $m^{(k)} = k - 1/2$. It follows that the

eigenvalues of B are

$$\begin{aligned} b^{(k)} &= 2m^{(k)} \\ &= 2k - 1. \end{aligned} \quad (2.27)$$

We will also be interested in the matrix elements for the operators $J^{(1)}$ and $J^{(2)}$. These can most easily be obtained by writing them as unit step operators multiplied by their respective magnitudes. This is analogous to the property that a vector in Euclidean space can always be written as a unit vector in the direction of the given vector multiplied by its magnitude. The unit step operators will be designated by θ_+ and θ_- with matrix elements

$$(\theta_+)_{jk} = \delta_{j, k+1}, \quad (\theta_-)_{jk} = \delta_{j+1, k} \quad (2.28)$$

The magnitude of $J^{(1)}$ and $J^{(2)}$ can be calculated from

$$|J^{(1)}| = (J^{(1)}\bar{J}^{(1)})^{\frac{1}{2}}, \quad (2.29)$$

$$|J^{(2)}| = (\bar{J}^{(2)}J^{(2)})^{\frac{1}{2}}, \quad (2.30)$$

where $\bar{J}^{(n)}$ denotes the adjoint of $J^{(n)}$, e.g., the adjoint of $J = a(q) + ib(q)p$ is $\bar{J} = a(q) - ipb(q)$. It can be shown that a relation between $\bar{J}^{(1)}$ and $J^{(2)}$ must exist,⁹ thus we conjecture

$$\bar{J}^{(1)} = J^{(2)} g(B). \quad (2.31)$$

Note that $J^{(1)}$ and $J^{(2)}$ are mutually adjoint only if $g(B) = 1$. This distinguishes these operators from the similar ones referred to in Section 1 where it was assumed such operators are mutually adjoint.

Now

$$\begin{aligned} J^{(1)} \bar{J}^{(1)} &= f(B)g(B) \\ &= [h^{(1)}(M-1)]^2, \end{aligned} \quad (2.32)$$

and

$$\begin{aligned} \bar{J}^{(2)} J^{(2)} &= f(B)/g(B) \\ &= [h^{(2)}(M-1)]^2, \end{aligned} \quad (2.33)$$

where $h^{(1)}$ and $h^{(2)}$ are introduced here for notational convenience.

We may therefore express the step operators in the form

$$J^{(1)} = h^{(1)}(M-1)\theta_+ = \theta_+ h^{(1)}(M), \quad (2.34)$$

$$J^{(2)} = \theta_- h^{(2)}(M-1) = h^{(2)}(M)\theta_-. \quad (2.35)$$

The matrix elements of $J^{(1)}$, $J^{(2)}$ are now clearly given by

$$(J^{(1)})_{jk} = \delta_{j, k+1} h^{(1)}(m(k)), \quad (2.36)$$

$$(J^{(2)})_{jk} = \delta_{j+1, k} h^{(2)}(m(j)). \quad (2.37)$$

For the operator $B = p^2 + q^2$ we have already determined that $f(B) = B - 1$. Also,

$$\bar{J}^{(1)} = q + ip = J^{(2)} \quad (2.38)$$

so that $g(B) = 1$, thus $J^{(1)}$ and $J^{(2)}$ are mutually adjoint in this particular case. We next resolve

$$\begin{aligned}
h^{(1)}(M-1) &= h^{(2)}(M-1) \\
&= (2M-1)^{\frac{1}{2}},
\end{aligned} \tag{2.39}$$

or replacing M by $M+1$

$$\begin{aligned}
h^{(1)}(M) &= h^{(2)}(M) \\
&= (2M+1)^{\frac{1}{2}}.
\end{aligned} \tag{2.40}$$

Consequently,

$$J^{(1)} = \theta_+ (2M+1)^{\frac{1}{2}}, \tag{2.41}$$

$$J^{(2)} = (2M+1)^{\frac{1}{2}} \theta_-, \tag{2.42}$$

so explicitly displaying the matrix elements we have

$$J^{(1)} = \begin{bmatrix} 0 & 0 & 0 & 0 & \dots \\ \sqrt{2} & 0 & 0 & 0 & \dots \\ 0 & \sqrt{4} & 0 & 0 & \dots \\ 0 & 0 & \sqrt{6} & 0 & \dots \\ 0 & 0 & 0 & \sqrt{8} & \dots \\ \dots & \dots & \dots & \dots & \dots \end{bmatrix}, \tag{2.43}$$

$$J^{(2)} = \begin{bmatrix} 0 & \sqrt{2} & 0 & 0 & 0 & \dots \\ 0 & 0 & \sqrt{4} & 0 & 0 & \dots \\ 0 & 0 & 0 & \sqrt{6} & 0 & \dots \\ 0 & 0 & 0 & 0 & \sqrt{8} & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \end{bmatrix}. \quad (2.44)$$

C. The Operators Γ and Δ

The operators Γ and Δ are not required to be self-adjoint although we will presume that Γ is positive-definite. The matrix representations of both operators can be handled similarly so that we will only display Δ in the following discussion.

We denote by $\Delta^{(0)}$ the diagonal matrix whose nonzero elements are identical with the center diagonal elements of Δ . Similarly, we denote by $\Delta^{(r)}\theta_{-}^r$ and $\theta_{+}^r\Delta^{(-r)}$ the matrices whose elements are identical with those of Δ in the r -th diagonal above and below the center diagonal respectively, and zero elsewhere. Hence

$$\Delta = \Delta^{(0)} + \sum_{r=1}^{\infty} (\theta_{+}^r\Delta^{(-r)} + \Delta^{(r)}\theta_{-}^r), \quad (2-45)$$

$$\Delta^{(r)} = \Delta^{(r)}(M),$$

with matrix elements

$$\Delta_{jk} = \Delta_j^{(0)} \delta_{jk} + \sum_{r=1}^{\infty} (\Delta_k^{(-r)} \delta_{j \ k+r} + \Delta_j^{(r)} \delta_{j+r \ k}), \quad (2.46)$$

$$\Delta_k^{(r)} = \Delta^{(r)}_{(m^{(k)})}.$$

Also we suppose that Δ can be represented as a function of $J^{(1)}$, $J^{(2)}$, and M ,

$$\Delta = E^{(0)} + \sum_{r=1}^{\infty} (J^{(1)r} E^{(-r)} + E^{(r)} J^{(2)r}), \quad (2.47)$$

$$E^{(r)} = E^{(r)}(M).$$

From Equations (2.34) and (2.35) it follows that

$$J^{(1)r} = \theta_+^r h^{(1)}(M) h^{(1)}(M+1) \dots h^{(1)}(M+r-1), \quad (2.48)$$

$$J^{(2)r} = h^{(2)}(M) h^{(2)}(M+1) \dots h^{(2)}(M+r-1) \theta_-^r, \quad (2.49)$$

so that upon comparison of (2.45) with (2.47) we identify

$$\Delta^{(0)} = E^{(0)}(M), \quad (2.50)$$

$$\Delta^{(-r)} = E^{(-r)}(M) h^{(1)}(M) h^{(1)}(M+1) \dots h^{(1)}(M+r-1), \quad (2.51)$$

$$\Delta^{(r)} = E^{(r)}(M) h^{(2)}(M) h^{(2)}(M+1) \dots h^{(2)}(M+r-1). \quad (2.52)$$

From these relations the matrix representation of appropriate perturbation terms can now be obtained. This is explicitly illustrated in Section 3.

D. The Operator Z

There is an inherent difficulty present in the form of the operator Z that does not occur for the linear operators, viz., it is a function of the unknown perturbed eigenvectors $\psi^{(k)}$. However, this difficulty can be alleviated by applying the same techniques characteristic of the standard theory. It is assumed that $\psi^{(k)}$ is a continuous function of the parameter α (when such a parameter does not explicitly appear in the eigenequation it can be introduced and later set equal to one) so that we can form the Taylor expansion about $\alpha = 0$,

$$\psi^{(k)}(\alpha) = \phi^{(k)} + \alpha \psi_1^{(k)} + \dots, \quad (2.53)$$

where $\psi_1^{(k)}$ is the derivative of $\psi^{(k)}$ with respect to α , evaluated at $\alpha = 0$, and $\phi^{(k)}$ is a normalized eigenvector of the operator B. Assuming that Z is analytic we may also expand it about $\alpha = 0$,

$$Z(\alpha, \psi^{(k)}) = Y + \alpha Z_1 + \dots, \quad (2.54)$$

where we define

$$Y = Z(0, \phi^{(k)}), \quad (2.55)$$

and

$$Z_1 = \left. \frac{\partial Z}{\partial \psi^{(k)}} \psi_1^{(k)} \right|_{\alpha=0}. \quad (2.56)$$

For first-order perturbations we shall henceforth approximate the operator Z by Y. The validity of such an approximation will, of course, depend on the convergence properties of (2.54).

From (2.55) we note the dependence of Y on the index k.

Since this index will refer to the k -th column in the matrix representation, we must calculate the matrix elements of Y by columns, i.e., for each column, Y is essentially a different operator. It is this column selection for the matrix elements of Y that constitutes the primary function of the operator $\bar{V}(q)$ defined in the Introduction. For present purposes we have absorbed this operator in the expansion (2.54).

The operator Y can be represented in a manner analogous to that for Δ . We shall denote by $Y^{(0)}$, $\theta_+^r Y^{(-r)}$, and $Y^{(r)} \theta_-^r$ matrices similar to those defined by the corresponding expressions containing the operator Δ . Thus we write

$$Y = Y^{(0)} + \sum_{r=1}^{\infty} (\theta_+^r Y^{(-r)} + Y^{(r)} \theta_-^r), \quad (2.57)$$

$$Y^{(r)} = Y^{(r)}_{(M)},$$

with matrix elements

$$Y_{jk} = Y_j^{(0)} \delta_{jk} + \sum_{r=1}^{\infty} (Y_k^{(-r)} \delta_{j, k+r} + Y_j^{(r)} \delta_{j+r, k}), \quad (2.58)$$

$$Y_j^{(r)} = Y^{(r)}_{(m^{(j)})}.$$

Also if we assume that Y , like Δ , can be expressed as a function of $J^{(1)}$, $J^{(2)}$, and M , then

$$Y = E^{(0)} + \sum_{r=1}^{\infty} (J^{(1)r} E^{(-r)} + E^{(r)} J^{(2)r}) \quad (2.59)$$

which, with the aid of Equations (2.48) and (2.49), allows us to make the associations

$$Y^{(0)} = E^{(0)}_{(M)}, \quad (2.60)$$

$$Y^{(-r)} = E^{(-r)}_{(M)} h^{(1)}_{(M)} h^{(1)}_{(M+1)} \dots h^{(1)}_{(M+r-1)}, \quad (2.61)$$

$$Y^{(r)} = E^{(r)}_{(M)} h^{(2)}_{(M)} h^{(2)}_{(M+1)} \dots h^{(2)}_{(M+r-1)}. \quad (2.62)$$

Because of the operator $\bar{V}(q)$, the above representation must be repeated for each column of the matrix Y , but only those elements that occur in the given column need be calculated. For example, suppose that we wish to calculate the matrix elements in the third column of Y that correspond to $Y = \phi^{(3)}$. Utilizing the above Equations (2.57) - (2.62) we would obtain the matrix expression for $\phi^{(3)}$,

$$\phi^{(3)} = \begin{bmatrix} \phi_{11}^{(3)} & \phi_{12}^{(3)} & \phi_{13}^{(3)} & \phi_{14}^{(3)} & \dots \\ \phi_{21}^{(3)} & \phi_{22}^{(3)} & \phi_{23}^{(3)} & \phi_{24}^{(3)} & \dots \\ \phi_{31}^{(3)} & \phi_{32}^{(3)} & \phi_{33}^{(3)} & \phi_{34}^{(3)} & \dots \\ \phi_{41}^{(3)} & \phi_{42}^{(3)} & \phi_{43}^{(3)} & \phi_{44}^{(3)} & \dots \\ \dots & \dots & \dots & \dots & \dots \end{bmatrix}. \quad (2.63)$$

However, out of this matrix representation we only select those elements in the third column for the representation for Y . Therefore, it becomes unnecessary to calculate the remaining elements.

To help eliminate other unnecessary calculations in computing the matrix elements of Y we note that whenever the coordinate q has a

symmetric matrix representation then

$$\begin{aligned}
 & E^{(r)}_{(M)} h^{(2)}_{(M)} h^{(2)}_{(M+1)} \dots h^{(2)}_{(M+r-1)} \\
 & = E^{(-r)}_{(M)} h^{(1)}_{(M)} h^{(1)}_{(M+1)} \dots h^{(1)}_{(M+r-1)}. \quad (2.64)
 \end{aligned}$$

This property means that we need not calculate any of the coefficients of $J^{(2)r}$ in Equation (2.59), as utilization of the coefficients of $J^{(1)r}$ will determine all matrix elements in a given column.

3. A NONLINEAR LEGENDRE-LIKE EQUATION

A. Formulation

For the special case of Equation (1.3) when $\mu = \nu = 0$ we obtain the nonlinear Legendre-like equation

$$\left[\frac{d}{dx} (1 - x^2) \frac{d}{dx} + \alpha x^2 u_k + \lambda_k \right] u_k = 0, \quad (3.1)$$

which in operational form featuring p and q becomes

$$[p(1 - q^2)p - \alpha q^2 \bar{V}(q) \psi^{(k)} - \lambda^{(k)}] \psi^{(k)} = 0. \quad (3.2)$$

Expanding $\psi^{(k)}$ in a Taylor series about $\alpha = 0$ yields

$$\psi^{(k)} = \phi^{(k)} + \alpha \psi_1^{(k)} + \dots \quad (3.3)$$

where $\phi^{(k)}$ again represents the normalized eigenvectors of the unperturbed operator. Hence we may write

$$[p(1 - q^2)p - \alpha q^2 \bar{V}(q) (\phi^{(k)} + \alpha \psi_1^{(k)} + \dots) - \lambda^{(k)}] \psi^{(k)} = 0, \quad (3.4)$$

and, upon retention of linear terms only in α , we finally obtain

$$[p(1 - q^2)p - \alpha q^2 \bar{V}(q) \phi^{(k)} - \lambda^{(k)}] \psi^{(k)} = 0. \quad (3.5)$$

Thus we can identify the operators

$$\begin{aligned} B &= p(1 - q^2)p, \\ \Gamma &= 1, \\ \Delta &= -\alpha q^2, \\ Y &= \bar{V}(q) \phi^{(k)}. \end{aligned} \quad (3.6)$$

Next we must find the eigenvalues and eigenvectors of the unperturbed operator B , then the matrix representations of the operators Δ and Y can be constructed.

B. The Operator B

The unperturbed form of Equation (3.5) is given by

$$[p(1 - q^2)p - b^{(k)}]U^{(k)} = 0. \quad (3.7)$$

To determine the associated step operators $J^{(1)}$, $J^{(2)}$ it is convenient to select $J_1 = q$; then

$$\begin{aligned} [B, J_1] &= [p^2, q] - q^2[p^2, q] + 2iq[p, q] \\ &= -2i(1 - q^2)p + 2q \\ &= 2(J_1 + J_2), \end{aligned} \quad (3.8)$$

$$\begin{aligned} [B, J_2] &= \{-ip(1 - q^2) + i(1 - q^2)p\} p(1 - q^2)p \\ &= i[p, q^2]p(1 - q^2)p \\ &= 2J_1B, \end{aligned} \quad (3.9)$$

where $J_2 = -i(1 - q^2)p$. The eigenvalues of the matrix c_{jk} are $\Lambda^{(1)} = 1 + (1 + 4B)^{1/2}$, $\Lambda^{(2)} = 1 - (1 + 4B)^{1/2}$. To avoid the square root we set $B = M(M + 1)$ so that $\Lambda^{(1)} = 2(M + 1)$ and $\Lambda^{(2)} = -2M$. The right-eigenvectors of c_{jk} are $\xi^{(1)} = (M + 1, 1)$, $\xi^{(2)} = (M, -1)$, hence

$$J^{(1)} = q(M + 1) - i(1 - q^2)p, \quad (3.10)$$

$$J^{(2)} = qM + i(1 - q^2)p, \quad (3.11)$$

where we have made use of Equation (2.8).

Now

$$\begin{aligned}
 f(B) &= J^{(1)}J^{(2)} \\
 &= [q(M + 1) - i(1 - q^2)p]J^{(2)} \\
 &= qJ^{(2)}M - i(1 - q^2)pJ^{(2)} \\
 &= q^2M^2 + iq(1 - q^2)pM - i(1 - q^2)pqM \\
 &\quad + (1 - q^2)p(1 - q^2)p \\
 &= M^2 - (1 - q^2)M(M + 1) + (1 - q^2)p(1 - q^2)p \\
 &= M^2, \tag{3.12}
 \end{aligned}$$

from which we conclude the first eigenvalue of M is $m^{(1)} = 0$.

Therefore, $m^{(k)} = k - 1$ and by applying the relation $b^{(k)} = m^{(k)}(m^{(k)} + 1)$ we then have

$$b^{(k)} = k(k - 1). \tag{3.13}$$

The first eigenvector $U^{(1)}$ satisfies

$$J^{(2)}U^{(1)} = 0, \tag{3.14}$$

or in differential equation form

$$(1 - x^2)\frac{dv_1}{dx} = 0, \tag{3.15}$$

where v_1 corresponds to the unperturbed eigenfunction. Therefore, $v_1 = \text{constant}$ is a solution of (3.15). Successive eigenvectors are determined from

$$U^{(k+1)} = J^{(1)}U^{(k)}, \tag{3.16}$$

which in differential equation form becomes

$$\begin{aligned} v_{k+1} &= [(k+1)x + (x^2 - 1) \frac{d}{dx}]^k v_1 \\ &= C_k \frac{d^k}{dx^k} (x^2 - 1)^k, \end{aligned} \quad (3.17)$$

where the C_k 's are constants. Normalization of the eigenfunctions v_k yields

$$v_k(x) = (k - \frac{1}{2})^{\frac{1}{2}} P_{k-1}(x), \quad (3.18)$$

where $P_k(x) = \frac{1}{2^k k!} \frac{d^k}{dx^k} (x^2 - 1)^k$ are the well-known Legendre polynomials.¹⁷ The normalized eigenvectors of (3.7) are then given by

$$\phi^{(k)} = (k - \frac{1}{2})^{\frac{1}{2}} P_{k-1}(q). \quad (3.19)$$

The function $g(B)$ is easily determined from the relation

$$\bar{J}^{(1)} = J^{(2)} g(B). \quad (3.20)$$

We have

$$\begin{aligned} \bar{J}^{(1)} &= (M+1)q + ip(1 - q^2) \\ &= (M+1)q + i(1 - q^2)p - 2q \\ &= (M-1)q + i(1 - q^2)p. \end{aligned} \quad (3.21)$$

From (3.10) and (3.11) it follows that

$$q = (J^{(1)} + J^{(2)})/(2M+1) \quad (3.22)$$

and

$$-i(1 - q^2)p = [J^{(1)}M - J^{(2)}(M+1)]/(2M+1). \quad (3.23)$$

Inserting (3.22) and (3.23) into Equation (3.21) gives

$$\begin{aligned}
 \bar{J}^{(1)} &= (M - 1)(J^{(1)} + J^{(2)})/(2M + 1) - [J^{(1)}_M - J^{(2)}(M + 1)]/(2M + 1) \\
 &= [J^{(1)}_M + J^{(2)}(M - 2) - J^{(1)}_M + J^{(2)}(M + 1)]/(2M + 1) \\
 &= J^{(2)}(2M - 1)/(2M + 1),
 \end{aligned} \tag{3.24}$$

from which we see that

$$g(B) = (2M - 1)/(2M + 1). \tag{3.25}$$

Thus

$$\begin{aligned}
 h^{(1)}(M - 1) &= [f(B)g(B)]^{\frac{1}{2}} \\
 &= M(2M - 1)^{\frac{1}{2}}/(2M + 1)^{\frac{1}{2}}
 \end{aligned} \tag{3.26}$$

and

$$\begin{aligned}
 h^{(2)}(M - 1) &= [f(B)/g(B)]^{\frac{1}{2}} \\
 &= M(2M + 1)^{\frac{1}{2}}/(2M - 1)^{\frac{1}{2}}.
 \end{aligned} \tag{3.27}$$

Summarizing results for the operator B we have:

$$(a). \quad B = p(1 - q^2)p, \quad \eta = 1$$

$$(b). \quad B = M(M + 1)$$

$$(c). \quad J_1 = q = (J^{(1)} + J^{(2)})/(2M + 1)$$

$$J_2 = -i(1 - q^2)p$$

$$= [J^{(1)}_M - J^{(2)}(M + 1)]/(2M + 1)$$

$$(d). \quad f(B) = M^2, \quad g(B) = (2M - 1)/(2M + 1)$$

$$(e). \quad m^{(k)} = k - 1, \quad b^{(k)} = k(k - 1)$$

$$(f). \quad \phi^{(k)} = (k - \frac{1}{2})^{\frac{1}{2}} P_{k-1}(q)$$

$$(g). \quad h^{(1)}(M) = (M + 1)(2M + 1)^{\frac{1}{2}} / (2M + 3)^{\frac{1}{2}}$$

$$h^{(2)}(M) = (M + 1)(2M + 3)^{\frac{1}{2}} / (2M + 1)^{\frac{1}{2}}$$

$$(h). \quad J^{(2)} J^{(1)} = h^{(2)}(M) h^{(1)}(M) = (M + 1)^2$$

C. Matrix Representation for Δ

The matrix representation for $\Delta = -\alpha q^2$ can readily be obtained from the expression

$$\begin{aligned} q^2 = & M^2 [(2M + 1)(2M - 1)]^{-1} + (M + 1)^2 [(2M + 1)(2M + 3)]^{-1} \\ & + J^{(1)2} [(2M + 1)(2M + 3)]^{-1} + [(2M + 3)(2M + 5)]^{-1} J^{(2)2}, \end{aligned} \quad (3.28)$$

derived by employing (c), (d), and (h) from the above list of properties. From Equation (2.47)

$$\Delta = E^{(0)} + \sum_{r=1}^{\infty} (J^{(1)r} E^{(-r)} + E^{(r)} J^{(2)r}) \quad (3.29)$$

so that we may also identify

$$E^{(0)}(M) = -\alpha \{ M^2 [(2M + 1)(2M - 1)]^{-1} + (M + 1)^2 [(2M + 1)(2M + 3)]^{-1} \} \quad (3.30)$$

$$E^{(-2)}(M) = -\alpha [(2M + 1)(2M + 3)]^{-1}, \quad (3.31)$$

$$E^{(2)}(M) = -\alpha [(2M + 3)(2M + 5)]^{-1}, \quad (3.32)$$

while all other $E^{(r)}(M)$ are zero. Hence, from Equations (2.50) - (2.52) and

$$h^{(1)}(M) = (M + 1) [(2M + 1)/(2M + 3)]^{\frac{1}{2}}, \quad (3.33)$$

$$h^{(2)}(M) = (M + 1) [(2M + 3)/(2M + 1)]^{\frac{1}{2}}, \quad (3.34)$$

we have upon simplification

$$\Delta^{(0)}(M) = -\alpha (2M^2 + 2M - 1) [(2M - 1)(2M + 3)]^{-1}, \quad (3.35)$$

$$\begin{aligned} \Delta^{(-2)}(M) &= \Delta^{(2)}(M) \\ &= -\alpha (M + 1)(M + 2) [(2M + 1)(2M + 3)^2(2M + 5)]^{-\frac{1}{2}}. \end{aligned} \quad (3.36)$$

Since $m^{(k)} = k - 1$, we obtain for the matrix elements

$$\Delta_{jk} = \Delta^{(0)}(m(j)) \delta_{jk} + \Delta^{(-2)}(m(k)) \delta_{j, k+2} + \Delta^{(2)}(m(j)) \delta_{j+2, k} \quad (3.37)$$

or finally

$$\Delta_{kk} = -\frac{\alpha}{2} (k^2 - k - \frac{1}{2}) / [(k + \frac{1}{2})(k - \frac{3}{2})], \quad (3.38)$$

$$\begin{aligned} \Delta_{k, k+2} &= \Delta_{k+2, k} \\ &= -\frac{\alpha}{4} k(k + 1) / [(k + \frac{1}{2})^2 (k - \frac{1}{2})(k + \frac{3}{2})]^{\frac{1}{2}}, \end{aligned} \quad (3.39)$$

and all other $\Delta_{jk} = 0$.

D. Matrix Representation for Y

The results of the two preceding sections are among those tabulated for linear operators by Green and Triffet.⁹ However, by making use of the relation $q = (J^{(1)} + J^{(2)})/(2M + 1)$ we can now extend these results to include certain nonlinear operators by formulating the normalized eigenvectors of the operator B as functions of $J^{(1)}$, $J^{(2)}$, and M, i.e.,

$$\phi^{(1)} = (1/2)^{\frac{1}{2}}, \quad (3.40)$$

$$\begin{aligned} \phi^{(2)} &= (3/2)^{\frac{1}{2}} q \\ &= (3/2)^{\frac{1}{2}} (J^{(1)} + J^{(2)})/(2M + 1), \end{aligned} \quad (3.41)$$

$$\begin{aligned} \phi^{(3)} &= \frac{1}{2} (5/2)^{\frac{1}{2}} (3q^2 - 1) \\ &= \frac{1}{2} (5/2)^{\frac{1}{2}} \{3[(J^{(1)} + J^{(2)})/(2M + 1)]^2 - 1\}, \end{aligned} \quad (3.42)$$

.

Keeping in mind that the matrix elements for Y must be calculated by columns as determined by $\bar{V}(q)$, we have for the first column ($Y = \phi^{(1)}$)

$$E^{(0)}(M) = (1/2)^{\frac{1}{2}}. \quad (3.43)$$

Therefore

$$E^{(0)}(0) = (1/2)^{\frac{1}{2}} \quad (3.44)$$

and the only nonzero matrix element in this column is

$$Y_{11} = (1/2)^{\frac{1}{2}}. \quad (3.45)$$

For the second column ($Y = \phi^{(2)}$)

$$\begin{aligned} E^{(0)}(M) &= 0, \\ E^{(-1)}(M) &= (3/2)^{\frac{1}{2}}/(2M + 1), \end{aligned} \quad (3.46)$$

so that by Equations (2.57) - (2.62) the only nonzero matrix elements must be

$$\begin{aligned} Y_{12} &= E^{(-1)}(0)h^{(1)}(0) \\ &= (1/2)^{\frac{1}{2}}, \end{aligned} \quad (3.47)$$

$$\begin{aligned} Y_{22} &= E^{(0)}(1) \\ &= 0, \end{aligned} \quad (3.48)$$

$$\begin{aligned} Y_{32} &= E^{(-1)}(1)h^{(1)}(1) \\ &= \frac{2}{5} (5/2)^{\frac{1}{2}}. \end{aligned} \quad (3.49)$$

For the third column

$$\begin{aligned} Y &= \phi^{(3)} \\ &= \frac{3}{2} (5/2)^{\frac{1}{2}} \{ M^2 [(2M + 1)(2M - 1)]^{-1} + (M + 1)^2 [(2M + 1)(2M + 3)]^{-1} - \frac{1}{3} \\ &\quad + J^{(1)2} [(2M + 1)(2M + 3)]^{-1} + [(2M + 3)(2M + 5)]^{-1} J^{(2)2} \}. \end{aligned} \quad (3.50)$$

Thus

$$E^{(0)}(M) = \frac{3}{2} (5/2)^{\frac{1}{2}} \{ M^2 [(2M + 1)(2M - 1)]^{-1}$$

$$\begin{aligned}
& + (M + 1)^2 [(2M + 1)(2M + 3)]^{-1} - \frac{1}{3}\}, \\
E^{(-2)}(M) &= \frac{3}{2} (5/2)^{\frac{1}{2}} [(2M + 1)(2M + 3)]^{-1}, \tag{3.51}
\end{aligned}$$

and the matrix elements become

$$\begin{aligned}
Y_{13} &= E^{(-2)}(0)h^{(1)}(0)h^{(1)}(1) \\
&= (1/2)^{\frac{1}{2}}, \tag{3.52}
\end{aligned}$$

$$\begin{aligned}
Y_{33} &= E^{(0)}(2) \\
&= \frac{2}{7} (5/2)^{\frac{1}{2}}, \tag{3.53}
\end{aligned}$$

$$\begin{aligned}
Y_{53} &= E^{(-2)}(2)h^{(1)}(2)h^{(1)}(3) \\
&= \frac{6}{7} (1/2)^{\frac{1}{2}}. \tag{3.54}
\end{aligned}$$

Again, the elements not listed in a given column are to be taken as zero. Following the same procedure for $\phi^{(4)}$, $\phi^{(5)}$, ..., will determine as many columns of Y as may be needed.

E. Summary of Results

The first few matrix elements calculated for B , Δ , and Y as they appear in the nonlinear Legendre-like equation (3.1) are displayed below:

$$B = \begin{bmatrix} 0 & 0 & 0 & 0 & \dots \\ 0 & 1 & 0 & 0 & \dots \\ 0 & 0 & 6 & 0 & \dots \\ 0 & 0 & 0 & 12 & \dots \\ \dots & \dots & \dots & \dots & \dots \end{bmatrix}, \tag{3.55}$$

$$\Delta = -\alpha \begin{bmatrix} 1/3 & 0 & 2/3\sqrt{5} & \dots \\ 0 & 3/5 & 0 & \dots \\ 2/3\sqrt{5} & 0 & 11/21 & \dots \\ \dots & \dots & \dots & \dots \end{bmatrix}, \quad (3.56)$$

$$Y = \begin{bmatrix} 1/\sqrt{2} & 1/\sqrt{2} & 1/\sqrt{2} & \dots \\ 0 & 0 & 0 & \dots \\ 0 & 2/\sqrt{10} & 2\sqrt{5}/7\sqrt{2} & \dots \\ 0 & 0 & 0 & \dots \\ 0 & 0 & 6/7\sqrt{2} & \dots \\ \dots & \dots & \dots & \dots \end{bmatrix}. \quad (3.57)$$

Combining these results gives the desired matrix representation for A ,

$$A_{jk} = b^{(j)}_{jk} \delta_{jk} + \sum_n \Delta_{jn} Y_{nk}. \quad (3.58)$$

A FORTRAN program, described in the Appendix, was used to find the eigenvalues and eigenvectors of the resulting nonsymmetric matrix. The eigenvalues corresponding to $\alpha = 1$ were computed by truncating A to 10 rows and columns. These are listed in Table 1, along with comparable values computed by the standard perturbation method as presented, for example, by Saaty and Bram.²

The reason that every other value agrees exactly is that the nondiagonal elements of A are zero for every other row, hence the diagonal element is itself an eigenvalue. This is a peculiarity of the particular matrix being considered. The difference in the other

Table 1. A comparison of eigenvalues for Equation (3.1) obtained by standard and matrix perturbation methods with $\alpha = 1$.

Standard Method		Matrix Method	
k	$\lambda(k)$	k	$\lambda(k)$
1	- 0.23570	1	- 0.24990
2	2.0000	2	2.0000
3	5.3977	3	5.3943
4	12.000	4	12.000
5	19.631	5	19.638
6	30.000	6	30.000
7	41.703	7	41.709
8	56.000	8	56.000
9	71.744	9	71.750
10	90.000	10	90.000

eigenvalues can be accounted for by the fact that standard perturbation theory presumes that the matrix A is essentially a diagonal matrix from the beginning, i.e., all nondiagonal elements are either zero or negligible in comparison with the diagonal elements. For such a matrix the eigenvalues can be approximated by the diagonal elements themselves. To assure that the nondiagonal elements are small conventional theory requires that the perturbation parameter α be small, thus forcing the desired condition. When $\alpha = 1$ the nondiagonal elements of the matrix (3.58) are relatively small so that the two methods of computing eigenvalues give nearly the same results. But, as α increases in magnitude a great deal more error is introduced by neglecting these nondiagonal elements of A .

To present a qualitative comparison of the two methods we shall examine how accurately the eigenvalues and eigenfunctions satisfy the original equation. The first eigenvalue and eigenfunction ($k = 1$)

computed by the standard theory are

$$\lambda_1 = - 0.23570 \quad (3.59)$$

and

$$u_1(x) = v_1(x) + 0.0351 v_3(x), \quad (3.60)$$

where $v_k(x)$ is defined by Equation (3.18). Substituting these expressions into Equation (3.1) yields the inequality

$$\left| \frac{d}{dx} (1 - x^2) \frac{du}{dx} + \lambda_1 u + x^2 u^2 \right| \leq 0.069, \quad |x| \leq 1, \quad (3.61)$$

whereas an exact solution would reduce the right-hand side to zero.

The corresponding eigenvalue and eigenfunction for the matrix method are

$$\lambda_1 = - 0.24990 \quad (3.62)$$

and

$$u_1(x) \approx v_1(x) + 0.0374 v_3(x) + 0.0008 v_5(x) + 0.0001 v_7(x). \quad (3.63)$$

Substituting these values into Equation (3.1) yields

$$\left| \frac{d}{dx} (1 - x^2) \frac{du}{dx} + \lambda_1 u + x^2 u^2 \right| \leq 0.004, \quad |x| \leq 1. \quad (3.64)$$

Equation (3.60) has been limited to the sum of two unperturbed eigenfunctions because that is all the standard theory predicts. On the other hand, the matrix method generates an infinite series of terms, the first four of which have been used for this calculation.

To provide an example where the perturbation term dominates the remaining linear terms we have chosen the case where $\alpha = 5$.

Table 2 contains the eigenvalues obtained by truncating A to 25 rows

and columns. Substituting the first eigenvalue and eigenfunction computed into Equation (3.1) gives

$$\left| \frac{d}{dx} (1 - x^2) \frac{du}{dx} + \lambda_1 u + 5x^2 u^2 \right| \leq 0.44, \quad |x| \leq 1. \quad (3.65)$$

This represents substantially more error than for the case when $\alpha = 1$, but it still may be considered a fair approximation for a first-order perturbation. No attempt at comparison with standard perturbation theory is made, since the latter is not expected to give even a qualitative solution for such a large perturbation.

In general the amount of error will increase with an increase in the magnitude of α . Additionally, for the nonlinear theory a significant amount of this error can be introduced when we approximate equations like (3.2) with equations like (3.5). No similar approximation occurs in the linear perturbation theory, and it is this point that most clearly sets the one apart from the other.

Table 2. Eigenvalues for the matrix given in Equation (3.58) with $\alpha = 5$.

k	$\lambda(k)$	k	$\lambda(k)$
1	- 1.6896	14	182.00
2	2.0000	15	209.04
3	3.0686	16	240.00
4	12.000	17	271.08
5	18.309	18	306.00
6	30.000	19	341.07
7	40.591	20	380.00
8	56.000	21	418.97
9	70.758	22	462.00
10	90.000	23	504.78
11	108.88	24	552.00
12	132.00	25	598.51
13	154.97		

4. GENERAL NONLINEAR SPECIAL-FUNCTION OPERATORS

A more generalized form of the nonlinear Legendre-like equation, as well as other types of nonlinearities, may appropriately be treated by the perturbation method. It is not essential to restrict considerations to equations of the special-function type, but when other kinds of equations are featured expressions like (1.1) generally must be used for computing the matrix elements. This can sometimes result in a computational disadvantage.

A. A Nonlinear Hypergeometric-like Equation

Again consider the nonlinear hypergeometric-like equation introduced in Section 1,

$$\left[\frac{d}{dx} (1 - x^2) \frac{d}{dx} - 2(\mu + \nu x) \frac{d}{dx} + \alpha x^2 u_k + \lambda_k \right] u_k = 0. \quad (4.1)$$

For first-order perturbations the operational form becomes

$$[p(1 - q^2)p + 2i(\mu + \nu q)p - \alpha q^2 \bar{V}(q) \phi^{(k)} - \lambda^{(k)}] \psi^{(k)} = 0 \quad (4.2)$$

with

$$\begin{aligned} B &= p(1 - q^2)p + 2i(\mu + \nu q)p, \\ \Gamma &= 1, \\ \Delta &= -\alpha q^2, \\ Y &= \bar{V}(q) \phi^{(k)}. \end{aligned} \quad (4.3)$$

Since most of the special-function equations can be obtained from the hypergeometric equation we feature it as a general example, the results of which may be applied to many other equations through appropriate transformations.

Following procedures similar to those of the last section we can obtain for the unperturbed operator B the relations

$$B = p(1 - q^2)p + 2i(\mu + \nu q)p,$$

$$\eta = (1 - q)^{-(\mu+\nu)}(1 + q)^{-(\nu-\mu)},$$

$$B = (M - \nu)(M + \nu + 1),$$

$$J_1 = q = (J^{(1)} + J^{(2)})/(2M + 1) - \mu\nu/[M(M + 1)],$$

$$J_2 = -i(1 - q^2)p$$

$$= [J^{(1)}(M - \nu) - J^{(2)}(M + \nu + 1)]/(2M + 1)$$

$$+ \mu(M - \nu)(M + \nu + 1)/[M(M + 1)],$$

$$f(B) = M^2 + \mu^2\nu^2/M^2 - \mu^2 - \nu^2,$$

$$g(B) = (2M - 1)/(2M + 1),$$

$$b^{(k)} = (m^{(1)} + k + \nu)(m^{(1)} + k - \nu - 1),$$

$$\text{where } m^{(1)2} + \mu^2\nu^2/m^{(1)2} = \mu^2 + \nu^2.$$

Details of computing the matrix elements of Δ and Y will be omitted since they are analogous to those given in Section 3. To represent $\Delta = -\alpha q^2$, however, we note that

$$\begin{aligned} q^2 = & R_1(M) + J^{(1)2}R_2(M) + R_2(M + 1)J^{(2)2} \\ & + J^{(1)}R_3(M) + R_4(M)J^{(2)} \end{aligned} \quad (4.4)$$

where the following have been defined for notational convenience:

$$R_1(M) = f(B)/[(2M+1)(2M-1)] + h^{(2)}(M)h^{(1)}(M)/[(2M+1)(2M+3)] \\ + \mu^2\nu^2/[M^2(M+1)^2], \quad (4.5)$$

$$R_2(M) = [(2M+1)(2M+3)]^{-1}, \quad (4.6)$$

$$R_3(M) = -\mu\nu\{[M(M+1)]^{-1} + [(M+1)(M+2)]^{-1}\}/(2M+1), \quad (4.7)$$

$$R_4(M) = -\mu\nu\{[M(M+1)]^{-1} + [(M+1)(M+2)]^{-1}\}/(2M+3). \quad (4.8)$$

Thus we identify

$$\Delta^{(0)} = -\alpha R_1(M), \quad (4.9)$$

$$\Delta^{(1)} = \Delta^{(-1)} \\ = -\alpha R_3(M)h^{(1)}(M), \quad (4.10)$$

$$\Delta^{(2)} = \Delta^{(-2)} \\ = -\alpha R_2(M)h^{(1)}(M)h^{(1)}(M+1). \quad (4.11)$$

By setting $M = m^{(k)}$, $m^{(k)} = m^{(1)} + k - 1$, we calculate the matrix elements

$$\Delta_{kk} = -\alpha R_1(m^{(k)}), \quad (4.12)$$

$$\Delta_{k \ k+1} = \Delta_{k+1 \ k} \\ = -\alpha R_3(m^{(k)})[m^{(k+1)2} + \mu^2\nu^2/m^{(k+1)2} - \mu^2 - \nu^2]^{\frac{1}{2}} \\ \times [(2m^{(k)} + 1)/(2m^{(k)} + 3)]^{\frac{1}{2}} \quad (4.13)$$

$$\begin{aligned}
\Delta_{k \ k+2} &= \Delta_{k+2 \ k} \\
&= -\alpha R_2(m^{(k)}) [m^{(k+1)2} + \mu^2 v^2 / m^{(k+1)2} - \mu^2 - v^2]^{\frac{1}{2}} \\
&\quad \times [m^{(k+2)2} + \mu^2 v^2 / m^{(k+2)2} - \mu^2 - v^2]^{\frac{1}{2}} \\
&\quad \times [(2m^{(k)} + 1) / (2m^{(k)} + 5)]^{\frac{1}{2}}.
\end{aligned} \tag{4.14}$$

All elements not listed are to be taken as zero.

For the operator Y we start by assuming that the normalized eigenvectors of B are of the polynomial form

$$\phi^{(k)} = \sum_{n=0}^N C_n^{(k)} q^n, \tag{4.15}$$

where the $C_n^{(k)}$ are constants. When this is not the case the eigenvectors can always be approximated by a polynomial through the use of a truncated Taylor series. For the first column ($Y = \phi^{(1)}$) we have

$$E^{(0)}(M) = C_0^{(1)} \tag{4.16}$$

so that the only nonzero element in the first column is

$$Y_{11} = C_0^{(1)}. \tag{4.17}$$

The second column has

$$\begin{aligned}
Y &= \phi^{(2)} \\
&= C_0^{(2)} + C_1^{(2)} q \\
&= C_0^{(2)} + C_1^{(2)} \{-\mu v / [M(M+1)] + J^{(1)}(2M+1)^{-1} \\
&\quad + (2M+3)^{-1} J^{(2)}\},
\end{aligned} \tag{4.18}$$

from which we identify

$$\begin{aligned} E^{(0)}(M) &= C_0^{(2)} - C_1^{(2)} \{ \mu\nu / [M(M+1)] \}, \\ E^{(-1)}(M) &= C_1^{(2)} (2M+1)^{-1}. \end{aligned} \quad (4.19)$$

Thus the matrix elements are

$$\begin{aligned} Y_{12} &= E^{(-1)}(m^{(1)}) h^{(1)}(m^{(1)}) \\ &= C_1^{(2)} [m^{(2)2} + \mu^2 \nu^2 / m^{(2)2} - \mu^2 - \nu^2]^{\frac{1}{2}} \\ &\quad \times [(2m^{(1)} + 1)(2m^{(1)} + 3)]^{-\frac{1}{2}}, \end{aligned} \quad (4.20)$$

$$\begin{aligned} Y_{22} &= E^{(0)}(m^{(2)}) \\ &= C_0^{(2)} - C_1^{(2)} [\mu\nu / m^{(2)} m^{(3)}], \end{aligned} \quad (4.21)$$

$$\begin{aligned} Y_{32} &= E^{(-1)}(m^{(2)}) h^{(1)}(m^{(2)}) \\ &= C_1^{(2)} [m^{(3)2} + \mu^2 \nu^2 / m^{(3)2} - \mu^2 - \nu^2]^{\frac{1}{2}} \\ &\quad \times [(2m^{(2)} + 1)(2m^{(2)} + 3)]^{-\frac{1}{2}}. \end{aligned} \quad (4.22)$$

Subsequent columns can be computed in the same manner.

B. Other Forms of Nonlinearity

Theoretically, matrix representations can be found for any nonlinear perturbation for which a Taylor series expansion like (2.54) exists. Listed below are more examples of nonlinear special-function operators illustrating certain other forms of nonlinearities. In addition to the first few matrix elements of the perturbations, we have tabulated the operator relationships essential for obtaining the matrix elements. Details of the calculations are omitted since they are analogous to those already presented.

1. Nonlinear Legendre-like Harmonics

$$\frac{d}{dx} (1 - x^2) \frac{du_k}{dx} + 2\alpha(1 - x^2) \frac{du_k}{dx} u_k + \lambda_k u_k = 0,$$

$$A = p(1 - q^2)p - i\alpha(1 - q^2)p\bar{V}(q)\phi^{(k)},$$

$$B = p(1 - q^2)p = M(M + 1),$$

$$\Gamma = 1,$$

$$\Delta = -i\alpha(1 - q^2)p,$$

$$Y = \bar{V}(q)\phi^{(k)},$$

$$q = (J^{(1)} + J^{(2)})/(2M + 1),$$

$$-i(1 - q^2)p = [J^{(1)}_M - J^{(2)}_{(M + 1)}]/(2M + 1),$$

$$f(B) = M^2, \quad g(B) = (2M - 1)/(2M + 1),$$

$$b^{(k)} = k(k - 1), \quad m^{(k)} = k - 1,$$

$$\phi^{(k)} = (k - \frac{1}{2})^{\frac{1}{2}} P_{k-1}(q),$$

where $P_j(q)$ is the j -th Legendre polynomial,

$$\Delta_{k+1 \ k} = \alpha k(k - 1)/[(2k - 1)(2k + 1)]^{\frac{1}{2}},$$

$$\Delta_{k \ k+1} = -\alpha k(k + 1)/[(2k - 1)(2k + 1)]^{\frac{1}{2}}.$$

The matrix elements of Y are exactly those given in Section 3 for the nonlinear Legendre-like equation discussed there.

2. Nonlinear Hermite-like Harmonics

$$\frac{d^2 u_k}{dx^2} - 2x \frac{du_k}{dx} + \alpha x u_k^3 + \lambda_k u_k = 0,$$

$$A = p^2 + 2iqp - \alpha q \bar{V}(q) \phi^{(k)2},$$

$$B = p^2 + 2iqp = 2M,$$

$$\Gamma = 1,$$

$$\Delta = -\alpha q,$$

$$Y = \bar{V}(q) \phi^{(k)2},$$

$$q = \frac{1}{2} (J^{(1)} + J^{(2)}),$$

$$ip = J^{(2)},$$

$$f(B) = 2M, \quad g(B) = 1,$$

$$b^{(k)} = 2(k-1), \quad m^{(k)} = k-1,$$

$$\phi^{(k)} = [2^{k-1} \pi^{\frac{1}{2}} (k-1)!]^{-\frac{1}{2}} H_{k-1}(q),$$

where $H_j(q)$ is the j -th Hermite polynomial,

$$\begin{aligned} \Delta_{k+1 \ k} &= \Delta_{k \ k+1} \\ &= -\alpha (k/2)^{\frac{1}{2}}, \end{aligned}$$

$$Y_{11} = (1/\pi)^{\frac{1}{2}}, \quad Y_{12} = 0, \quad \dots$$

$$Y_{21} = 0, \quad Y_{22} = (9/\pi)^{\frac{1}{2}}, \quad \dots$$

$$Y_{31} = 0, \quad Y_{32} = 0, \quad \dots$$

$$\dots, \quad \dots, \quad \dots$$

The above unperturbed operator $B = p^2 + 2iqp$ is related by a similarity transformation to the familiar harmonic oscillator operator $B' = p^2 + q^2$, which we have featured as an illustrative example in Section 2.

3. Nonlinear Laguerre-like Harmonics

$$x \frac{d^2 u_k}{dx^2} + (1-x) \frac{du_k}{dx} + \alpha x u_k \sin(u_k) + \lambda_k u_k = 0,$$

$$A = qp^2 - i(1-q)p - \alpha q \bar{V}(q) \sin(\phi^{(k)}),$$

$$B = qp^2 - i(1-q)p = M,$$

$$\Gamma = 1,$$

$$\Delta = -\alpha q,$$

$$Y = \bar{V}(q) \sin(\phi^{(k)}),$$

$$q = (J^{(1)} + J^{(2)}) + 2M + 1,$$

$$f(B) = M, \quad g(B) = 1,$$

$$b^{(k)} = k - 1, \quad m^{(k)} = k - 1,$$

$$\phi^{(k)} = L_{k-1}(q),$$

where $L_j(q)$ is the j -th Laguerre polynomial,

$$\Delta_{kk} = -\alpha(2k - 1),$$

$$\begin{aligned} \Delta_{k+1, k} &= \Delta_{k, k+1} \\ &= -\alpha k^{\frac{1}{2}}, \end{aligned}$$

$$Y_{11} = \sin (1), Y_{12} = \frac{1}{2} \sin (1), \quad \dots$$

$$Y_{21} = 0, \quad Y_{22} = 0, \quad \dots$$

$$Y_{31} = 0, \quad Y_{32} = -\frac{1}{2} \cos (1), \quad \dots$$

$$\dots, \quad \dots, \quad \dots$$

5. OTHER EXAMPLES

A. The Hartree Equations for the Helium Atom

The Hartree equations for the helium atom are classic examples of nonlinear equations arising because of the interactions between particles. They follow from applying the theory of the self-consistent field¹⁸ to the Hamiltonian

$$H = -(\nabla_1^2 + \nabla_2^2) - \frac{4}{r_1} - \frac{4}{r_2} + \frac{2\alpha}{r_{12}}, \quad (5.1)$$

where $\underline{r}_1$ and $\underline{r}_2$ are the coordinates of the two electrons relative to the nucleus, $r_{12} = r_{21}$ represents the distance between the electrons, and α is a parameter related to the strength of the Coulomb repulsion between the electrons. Spin-dependent forces are neglected.

The central-field postulate is the general principle underlying the Hartree self-consistent field. It is assumed that each electron moves independently of the other in a central potential representing the Coulomb potential of the nucleus and the averaged potential field of the remaining electron. Thus the time-independent wave function of the helium atom is written as

$$\psi(\underline{r}_1, \underline{r}_2) = u^{(1)}(\underline{r}_1)u^{(2)}(\underline{r}_2), \quad (5.2)$$

where

$$u^{(j)}(\underline{r}_j) \sim R_{nl}^{(j)}(r_j)Y_{lm}^{(j)}(\theta_j, \phi_j), \quad j = 1, 2 \quad (5.3)$$

designates the one-electron orbitals. Here r, θ, ϕ are the standard

spherical coordinates, the $Y_{\ell m}^{(j)}$ are the spherical harmonic functions¹⁷ and the $R_{n\ell}^{(j)}$ are radial functions.¹⁸

Applying the principles of the calculus of variations to the total energy of the atom we obtain the two nonlinear radial equations

$$\left[-\frac{d^2}{dr_j^2} + \frac{\ell(\ell+1)}{r_j^2} - \frac{4}{r_j} + \frac{2\alpha}{r_j} S(r, n, \ell) \right] P_{n\ell}^{(j)} = E_{n\ell}^{(j)} P_{n\ell}^{(j)}, \quad (5.4)$$

for $j = 1, 2$,

$$P_{n\ell}^{(j)}(r_j) = r_j R_{n\ell}^{(j)}(r_j), \quad (5.5)$$

and

$$S(r_j, n, \ell) = \int_0^{r_j} [P_{n\ell}^{(i)}(r_i)]^2 dr_i + \int_{r_j}^{\infty} [P_{n\ell}^{(i)}(r_i)]^2 \left(\frac{r_j}{r_i}\right) dr_i, \quad (5.6)$$

where $i = 1, 2$, but $i \neq j$.

When $\alpha = 0$ Equations (5.4) both become hydrogenic radial equations with the operational form

$$[p^2 + \ell(\ell+1)q^{-2} - 4q^{-1} - b^{(k)}]U^{(k)} = 0. \quad (5.7)$$

The operator $B = p^2 + \ell(\ell+1)q^{-2} - 4q^{-1}$ does not lend itself to the calculation of the step operators $J^{(1)}$ and $J^{(2)}$ as we have defined them. This is a consequence of the fact that the discrete eigenvalues of B are bounded above, as will soon be made clear. We consider the transformation

$$Q = (-b^{(k)})^{\frac{1}{2}} q, \quad P = (-b^{(k)})^{-\frac{1}{2}} p, \quad (5.8)$$

$QP - PQ = i$, which transforms the operator B to

$$B' = QP^2 + Q + \ell(\ell + 1)Q^{-1}, \quad (5.9)$$

with the associated eigenequation

$$B'U^{(k)} = 4(-b^{(k)})^{-\frac{1}{2}} U^{(k)}. \quad (5.10)$$

Hence, the eigenvectors of B' in the coordinate Q are the same as for B in the coordinate q . Following the procedure of Section 2 the step operators of B' are determined to be

$$J^{(1)} = Q - iQP - M, \quad (5.11)$$

$$J^{(2)} = Q + iQP - M. \quad (5.12)$$

Utilizing these we may obtain the relations

$$B' = 2M,$$

$$J_1 = Q = \frac{1}{2} (J^{(1)} + J^{(2)}) + M,$$

$$J_2 = -iQP = \frac{1}{2} (J^{(1)} - J^{(2)}),$$

$$f(B) = M(M - 1) - \ell(\ell + 1), \quad g(B) = 1,$$

$$b^{(k)} = 4(-b^{(k)})^{-\frac{1}{2}} = 2(k + \ell),$$

$$U^{(k)} = (2Q)^{\ell+1} e^{-Q} L_{n+\ell}^{2\ell+1}(2Q), \quad (5.13)$$

where $n = k + \ell$ and the $L_j^m(x)$ are generalized Laguerre polynomials.¹⁷

Thus, the eigenvalues and normalized eigenvectors of B are given by



$$b^{(k)} = -4/n^2, \quad n = 1, 2, \dots, \quad (5.14)$$

$$\phi^{(k)} = \frac{\sqrt{2(n - \ell - 1)!}}{\sqrt{n^2[(n + \ell)!]^3}} \left(\frac{4q}{n}\right)^{\ell+1} e^{-2q/n} L_{n+\ell}^{2\ell+1}(4q/n). \quad (5.15)$$

The perturbing operators Δ and Y for Equations (5.4) also have similar forms defined by

$$\Delta = 2\alpha q^{-1}, \quad (5.16)$$

and

$$Y = \bar{V}(q)S(q, n, \ell). \quad (5.17)$$

Because the discrete eigenvalues $b^{(k)}$ have the upper limit zero the discrete eigenvectors $\phi^{(k)}$, of the operator B , do not form a complete system of orthonormal vectors.¹⁴ Therefore, as suggested above, they do not provide a suitable basis for a matrix representation. The eigenvectors associated with the operator B' do form a complete orthonormal system, however, and it is this set that we shall utilize for our matrix representations, even though the operator B will no longer be diagonal.

To calculate the ground state energy of the helium atom we seek to diagonalize the matrix

$$A = B + \Delta Y, \quad (5.18)$$

where B represents the energy of one electron due only to the Coulomb potential of the nucleus and ΔY expresses the energy of interaction of the electrons. To the first eigenvalue of A must be added the energy

$b^{(1)}$ of the other electron due to the potential of the nucleus alone. Our matrix representation will be based upon the condition that $\ell = 0$ even though this is not entirely correct whenever $n > 1$; there is a degeneracy in the ℓ quantum number but the major contribution to the energy occurs for $\ell = 0$. Also for $\ell = 0$, the operator Y can be approximated by¹⁸

$$Y = 1 - (1 + 2q/n)e^{-4q/n}. \quad (5.19)$$

Because the form of the perturbation does not lend itself to the operator method of computing matrix elements in this case we have utilized an analytical technique, a general discussion of which is presented in Section 6. The matrix representations for B and ΔY can then be defined by

$$B_{jk} = \int_0^\infty \phi^{(j)} B \phi^{(k)} dq \quad (5.20)$$

and

$$(\Delta Y)_{jk} = 2\alpha \int_0^\infty \phi^{(j)} q^{-1} S(q, k, 0) \phi^{(k)} dq, \quad (5.21)$$

where $\phi^{(k)}$ represents the normalized eigenvectors of the operator B' . To be explicit, the first matrix elements of (5.20) and (5.21) are given by ($\alpha = 1$),

$$\begin{aligned} B_{11} &= -4 \int_0^\infty e^{-2q}(q^2 + 2q) dq \\ &= -3, \end{aligned} \quad (5.22)$$

$$\begin{aligned}
 (\Delta Y)_{11} &= 8 \int_0^{\infty} [e^{-2q}q - e^{-6q}(2q^2 + q)] dq \\
 &\approx 1.6296.
 \end{aligned}
 \tag{5.23}$$

Continued calculations will finally yield the representations

$$B = \begin{bmatrix} -3.0000 & 1.1550 \\ 1.1550 & -1.6667 \end{bmatrix}, \tag{5.24}$$

and

$$\Delta Y = \begin{bmatrix} 1.6296 & -0.3512 \\ -0.6842 & 1.0000 \end{bmatrix}. \tag{5.25}$$

The first eigenvalue of $A = B + \Delta Y$ is

$$E_{10}^{(1)} = -1.724 \text{ Rydbergs}, \tag{5.26}$$

so that the total ground state energy becomes

$$\begin{aligned}
 E_{10} &= E_{10}^{(1)} + b^{(1)} \\
 &= -5.724 \text{ Rydbergs}.
 \end{aligned}
 \tag{5.27}$$

Compared with the experimental value of -5.807 Rydbergs, this represents an error of 0.083 Rydbergs. If larger matrix representations are desired, then the approximation (5.19) should probably not be used, as its validity beyond $n = 2$ is questionable. The calculation of Y from expressions like (5.6), however, is extremely tedious.

Millman and Keller¹⁹ have computed the ground state energy for the helium atom by applying a modified form of the standard perturbation method to the Hartree equations. They obtained a value of

- 5.500 Rydbergs, representing an error of 0.307 Rydbergs with the experimental value. In addition, they made a comparison of results with those achieved by applying conventional perturbation techniques to the Schrödinger equation and showed that the eigenvalues agree up to first-order terms, but that the eigenvectors agree only up to zero-order terms.

By the present method, however, it can easily be shown that the matrix representation for the (radial) Schrödinger equation, whose Hamiltonian is given by (5.1), becomes

$$H_T = 2B + \Delta Y, \quad (5.28)$$

where B , Δ , and Y are the same as defined for the Hartree equations and $\ell = 0$. Clearly, the eigenvalues of (5.28) will not yield the same values as for the Hartree equations since the sum of the eigenvalues of two matrices is not the same, in general, as the eigenvalues of the sum of the same two matrices.

B. The van der Pol Equation

An equation of frequent occurrence in the field of nonlinear oscillations is the van der Pol equation. A general form of this equation is given by

$$u'' - \alpha(1 - u^2)u' + \lambda u = 0, \quad \lambda > 0, \quad (5.29)$$

where the primes indicate derivatives with respect to time. Up to this point we have concentrated entirely on the problem of finding those values of the parameter λ for which nontrivial solutions of the

differential equation exist, subject to certain boundary conditions. In nonlinear oscillation theory equations such as (5.29) are treated as initial-value problems, where one seeks periodic solutions for a fixed value of λ . Because of this distinction, the matrix perturbation method featured here must be applied in a slightly different way.

To be precise, we look for solutions of (5.29) with $\lambda = 1$ satisfying

$$u(t + 2\pi/\omega) = u(t) \quad (5.30)$$

and subject to the initial conditions

$$u(0) = 2, \quad u'(0) = 0. \quad (5.31)$$

The existence of such solutions is guaranteed by the theorem of Liénard;²⁰ and stability requirements indicate that the amplitude of $u(t)$ varies between +2 and -2.

The unperturbed solution of (5.29) subject to the initial conditions (5.31) is given by

$$u_0(t) = 2 \cos \omega_0 t, \quad (5.32)$$

where $\omega_0 = \sqrt{\lambda} = 1$ is the angular frequency. The effect of the nonlinear term in the van der Pol equation is to change the angular frequency ω_0 to a new value ω , but we can calculate ω by expanding λ in a Taylor series about $\alpha = 0$,

$$\lambda = \omega_0^2 + \alpha \rho_1 + \dots, \quad (5.33)$$

then setting $\lambda = 1$ to obtain

$$\omega = \sqrt{1 - \alpha \rho_1}, \quad (5.34)$$

where $\alpha\rho_1$ represents the first-order perturbation in the eigenvalues of (5.29).

In order to obtain a complete set of eigenfunctions, from which appropriate matrix representations can be derived, we reformulate (5.29) as a boundary-value problem. Choosing $0 \leq t \leq \pi$ as the fundamental domain of the Hilbert space and imposing the boundary conditions

$$u(0) = 2, \quad u(\pi/\omega) = -2, \quad (5.35)$$

which are consistent with stability requirements and the initial conditions (5.31), then the eigenvalues and normalized eigenfunctions of the unperturbed equation are

$$b_k = k^2 \quad (5.36)$$

and

$$v_k(t) = C \cos kt, \quad C = \sqrt{2/\pi}, \quad (5.37)$$

respectively.

The nonlinear operator of (5.29) is identified as

$$N^0 = (1 - v_k^2) \frac{d}{dt} \quad (5.38)$$

to a first-order perturbation. To compute the matrix elements of N^0 it is again most convenient to apply the method discussed in Section 6. Thus, we write

$$N_{jk}^0 = -kC^2 \int_0^\pi [\cos jt(1 - C^2 \cos^2 kt) \sin kt] dt, \quad (5.39)$$

which upon evaluation yields

$$N_{kk}^0 = N_{3k k}^0 = 0, \quad (5.40)$$

and for $j \neq k$ or $3k$,

$$N_{jk}^0 = \frac{k^2 C^2}{4} [1 - (-1)^{j+k}] \left(\frac{4 - C^2}{j^2 - k^2} + \frac{3C^2}{9k^2 - j^2} \right), \quad (5.41)$$

where $C^2 = 2/\pi$.

Diagonalization of the matrix $A_{jk} = b_j \delta_{jk} + \alpha N_{jk}^0$ will produce an infinite set of eigenvalues $\lambda^{(k)}$ and associated eigenvectors, from which we can extract solutions to the van der Pol equation for all cases where the fixed parameter $\lambda = k^2$. The first eigenvalues are

$$\lambda^{(1)} = 1.0539 \quad (5.42)$$

and

$$\lambda^{(1)} = 1.2161 \quad (5.43)$$

for $\alpha = 0.5$ and $\alpha = 1$, respectively. From these, the first-order perturbations are determined to be

$$\alpha \rho_1 = 0.0539 \quad (5.44)$$

and

$$\alpha \rho_1 = 0.2161; \quad (5.45)$$

hence, by applying (5.34) the perturbed angular frequencies become

$$\omega = 0.9726 \quad (5.46)$$

and

$$\omega = 0.8854 \quad (5.47)$$

for $\alpha = 0.5$ and $\alpha = 1$.

Since in this case it has been specified that $\lambda = 1$, the desired solution can be expressed in the form

$$u(t) = D_0 + D_1 u^{(1)}(t), \quad (5.48)$$

where $u^{(1)}(t)$ is the perturbed eigenfunction belonging to the first eigenvalue $\lambda^{(1)}$, while D_0 and D_1 are two constants to be evaluated from the boundary conditions (5.35). Solutions corresponding to $\alpha = 0.5$ and $\alpha = 1.0$, respectively, are given by

$$\begin{aligned} u(t) \approx & 0.1599 + 1.9921 \cos \omega t - 0.1585 \cos 2\omega t \\ & + 0.0095 \cos 3\omega t + 0.0006 \cos 4\omega t \\ & + 0.0013 \cos 5\omega t - 0.0004 \cos 6\omega t \end{aligned} \quad (5.49)$$

and

$$\begin{aligned} u(t) \approx & 0.3121 + 1.9582 \cos \omega t - 0.3095 \cos 2\omega t \\ & + 0.0371 \cos 3\omega t - 0.0005 \cos 4\omega t \\ & + 0.0053 \cos 5\omega t - 0.0014 \cos 6\omega t \\ & - 0.0005 \cos 7\omega t - 0.0005 \cos 8\omega t, \end{aligned} \quad (5.50)$$

again retaining only the first few terms of the infinite series.

These solutions give values of $u(t)$ and $u'(t)$ which are comparable with those obtained through the use of time-consuming numerical

techniques.²⁰ This comparison is presented for half a period in Table 3; by periodic extension the entire solution can be constructed.

Attempts were made to obtain solutions for larger values of the parameter α , but it was discovered that the error in the perturbed angular frequency ω grew very rapidly for $\alpha > 1$. However, if one extended to second-order perturbations, qualitative results for larger

Table 3. Approximations of $u(t)$ and $u'(t)$ for the van der Pol equation obtained by numerical and matrix techniques.

$\alpha = 0.5$					$\alpha = 1.0$				
t	Numerical Method		Matrix Method		t	Numerical Method		Matrix Method	
	u(t)	u'(t)	u(t)	u'(t)		u(t)	u'(t)	u(t)	u'(t)
0.0	2.00	0.00	2.00	0.00	0.0	2.00	0.00	2.00	0.00
0.1	1.99	-0.19	1.99	-0.14	0.1	1.99	-0.17	1.99	-0.09
0.2	1.96	-0.34	1.97	-0.28	0.2	1.97	-0.30	1.98	-0.18
0.3	1.92	-0.48	1.93	-0.42	0.3	1.93	-0.40	1.96	-0.26
0.4	1.87	-0.60	1.89	-0.55	0.4	1.89	-0.47	1.93	-0.35
0.5	1.80	-0.71	1.82	-0.68	0.5	1.84	-0.53	1.89	-0.43
0.6	1.73	-0.80	1.75	-0.81	0.6	1.78	-0.59	1.85	-0.51
0.7	1.64	-0.89	1.66	-0.94	0.7	1.72	-0.64	1.79	-0.59
0.8	1.55	-0.98	1.56	-1.07	0.8	1.65	-0.68	1.73	-0.67
0.9	1.45	-1.07	1.45	-1.19	0.9	1.58	-0.73	1.66	-0.75
1.0	1.33	-1.15	1.33	-1.31	1.0	1.51	-0.78	1.58	-0.84
1.1	1.21	-1.24	1.19	-1.43	1.1	1.43	-0.83	1.49	-0.92
1.2	1.09	-1.34	1.04	-1.54	1.2	1.34	-0.89	1.39	-1.02
1.3	0.95	-1.44	0.88	-1.65	1.3	1.25	-0.96	1.28	-1.12
1.4	0.80	-1.54	0.71	-1.75	1.4	1.15	-1.04	1.17	-1.24
1.5	0.64	-1.65	0.53	-1.83	1.5	1.04	-1.12	1.04	-1.35
1.6	0.47	-1.77	0.35	-1.91	1.6	0.92	-1.23	0.89	-1.47
1.7	0.28	-1.88	0.15	-1.96	1.7	0.80	-1.35	0.74	-1.58
1.8	0.09	-2.00	-0.04	-2.00	1.8	0.65	-1.49	0.58	-1.69
1.9	-0.11	-2.10	-0.24	-2.01	1.9	0.50	-1.65	0.40	-1.78
2.0	-0.33	-2.18	-0.44	-2.00	2.0	0.32	-1.83	0.22	-1.86
2.1	-0.55	-2.22	-0.64	-1.97	2.1	0.13	-2.04	0.04	-1.91
2.2	-0.77	-2.22	-0.84	-1.91	2.2	-0.08	-2.25	-0.15	-1.94
2.3	-0.99	-2.15	-1.03	-1.83	2.3	-0.32	-2.46	-0.35	-1.95
2.4	-1.20	-2.02	-1.20	-1.72	2.4	-0.58	-2.62	-0.54	-1.94
2.5	-1.39	-1.83	-1.37	-1.59	2.5	-0.84	-2.68	-0.74	-1.91
2.6	-1.56	-1.58	-1.52	-1.43	2.6	-1.11	-2.59	-0.93	-1.85
2.7	-1.71	-1.29	-1.65	-1.25	2.7	-1.35	-2.34	-1.11	-1.77
2.8	-1.82	-1.00	-1.77	-1.05	2.8	-1.57	-1.95	-1.28	-1.67
2.9	-1.91	-0.71	-1.86	-0.82	2.9	-1.74	-1.48	-1.45	-1.54
3.0	-1.96	-0.43	-1.93	-0.59	3.0	-1.87	-1.02	-1.59	-1.38
3.1	-1.99	-0.19	-1.98	-0.33	3.1	-1.95	-0.62	-1.72	-1.19
3.2	-2.00	0.02	-2.00	-0.08	3.2	-1.99	-0.29	-1.83	-0.97
3.3	-1.99	0.20	-1.99	0.18	3.3	-2.00	-0.04	-1.91	-0.71
3.4	-1.96	0.36	-1.96	0.44	3.4	-2.00	0.14	-1.97	-0.44
3.5	-1.92	0.50	-1.91	0.68	3.5	-1.98	0.28	-2.00	-0.14

values of α could be obtained. Higher-order perturbations are discussed in Section 6, but extensive calculations would be required to yield the additional matrix elements.

As a final comment it could also be mentioned that the results given here for the van der Pol equation were calculated by treating only first-order perturbations, whereas for the standard method the second-order perturbation must be included before a change in angular frequency is detected.

6. GENERAL REMARKS

A. Higher-Order Perturbations

So far we have concerned ourselves only with first-order perturbation effects. For most of the applications we have in mind, where the nonlinear term is of the same order of magnitude as the linear terms ($\alpha = 1$), first-order corrections obtained by this particular method are probably sufficient. However, when the perturbing term becomes large in comparison to the other terms ($\alpha > 1$), a second-order correction to the unperturbed solution may be necessary in the interest of accuracy. This second-order correction will appear in the form of another operator added to A,

$$A = B + \Delta(Y + \Omega), \quad (6.1)$$

where B still designates the unperturbed linear operator, ΔY is the first-order nonlinear perturbation of B, and $\Delta\Omega$ represents the second-order perturbation. Here Γ is assumed to be unity, since it is not essential to the following discussion.

To obtain the explicit form of the operator Ω from which its matrix elements can be calculated, we reconsider the general nonlinear equation

$$(B + \Delta Z - \lambda^{(k)}) \psi^{(k)} = 0. \quad (6.2)$$

As before in Section 2(D) we expand the operator Z in a Taylor series about $\alpha = 0$,

$$Z = Y + \alpha Z_1 + \alpha^2 Z_2 + \dots, \quad (6.3)$$

where again

$$Z_1 = \left. \frac{\partial Z}{\partial \psi}^{(k)} \psi_1^{(k)} \right|_{\alpha=0}, \dots, \quad (6.4)$$

and insert this into Equation (6.2),

$$[B + \Delta(Y + \alpha Z_1 + \alpha^2 Z_2 + \dots) - \lambda^{(k)}] \psi^{(k)} = 0. \quad (6.5)$$

Retaining not only Y but also the term αZ_1 , Equation (6.5) becomes

$$[B + \Delta(Y + \alpha Z_1) - \lambda^{(k)}] \psi^{(k)} = 0, \quad (6.6)$$

so that $\Omega = \alpha Z_1$. Assuming the first-order perturbation problem to be solved, we will know $\psi_1^{(k)}$, hence Z_1 , and can therefore write

$$\Omega = \sum_{\ell \neq k} \gamma_{\ell}^{(k)} \phi_{\ell}^{(\ell)} \left. \frac{\partial Z}{\partial \psi}^{(k)} \right|_{\alpha=0}, \quad (6.7)$$

where $\gamma_{\ell}^{(k)}$ represents the vector components (normalized in such a way that $\gamma_k^{(k)} = 1$) of the eigenvectors $\psi^{(k)}$. In obtaining (6.7) we have used the expansion

$$\begin{aligned} \psi^{(k)} &= \phi^{(k)} + \alpha \psi_1^{(k)} \\ &= \phi^{(k)} + \sum_{\ell \neq k} \gamma_{\ell}^{(k)} \phi_{\ell}^{(\ell)} \end{aligned} \quad (6.8)$$

for the first-order terms. A matrix representation for Ω can now be obtained in a manner similar to that defined for Y . Hence, A can be expressed as

$$A_{jk} = b^{(j)} \delta_{jk} + \sum_n \Delta_{jn} (Y_{nk} + \Omega_{nk}). \quad (6.9)$$

There is, of course, one form of Z which simplifies some of the computations required to obtain the matrix elements of Ω . This occurs when $Z = \bar{V}(q)\psi^{(k)}$ so that

$$\Omega = \sum_{\ell \neq k} \gamma_{\ell}^{(k)} \bar{V}(q) \phi^{(\ell)}; \quad (6.10)$$

in particular,

$$\begin{aligned} \Omega_{1k} &= 0, \\ \Omega_{j1} &= \gamma_j^{(1)} / \sqrt{2}, \quad j \neq 1, \\ \Omega_{kk} &= \sum_{\ell \neq k} \gamma_{\ell}^{(k)} \gamma_{\ell k}. \end{aligned} \quad (6.11)$$

Some of the matrix elements of Ω for the nonlinear Legendre-like equation discussed in Section 3 are displayed below; for the case when $\alpha = 1$ we obtain:

$$\Omega = \begin{bmatrix} 0 & 0 & 0 & \dots \\ 0 & -0.0592 & 0 & \dots \\ 0.0264 & 0 & -0.0303 & \dots \\ \dots & \dots & \dots & \dots \end{bmatrix} \quad (6.12)$$

To compare the results of first-order to second-order perturbations we will treat 3×3 matrix representations for the nonlinear Legendre-like operator. The first eigenvalue and eigenfunction are

$$\lambda_1 = -0.2495$$

and

$$u_1(x) = v_1(x) + 0.0373 v_3(x),$$

for the first-order perturbation, while for the second-order perturbation obtained by diagonalizing (6.9),

$$\lambda_1 = - 0.2579$$

and

$$u_1(x) = v_1(x) + 0.0396 v_3(x).$$

Substituting these values into Equation (3.1) gives

$$\left| \frac{d}{dx} (1 - x^2) \frac{du_1}{dx} + \lambda_1 u_1 + x^2 u_1^2 \right| \leq 0.042, \quad |x| \leq 1$$

and

$$\left| \frac{d}{dx} (1 - x^2) \frac{du_1}{dx} + \lambda_1 u_1 + x^2 u_1^2 \right| \leq 0.018, \quad |x| \leq 1$$

for first-order and second-order perturbations, respectively.

Following similar procedures one can in principle define third-, fourth-, and higher-order perturbations. However, obtaining the matrix elements in such cases may well take too long to be practical.

B. Analytical Methods

As we have seen there are certain differential equations for which the operator technique of computing matrix elements is not convenient. In these cases the usual analytical method has been applied. Perhaps a few comments on the latter approach and its relation to the operator technique would be helpful.

Again consider the nonlinear equation (2.1),

$$(L + \alpha N + \lambda)u = 0. \tag{6.13}$$

Assuming that $u = u(x)$ is also a continuous function of α , we form the Taylor expansion about $\alpha = 0$,

$$u = u_0 + \alpha T_1 + \dots \quad (6.14)$$

where u_0 represents the unperturbed solution of Equation (6.13) and αT_1 is the first-order perturbation. Thus it follows that

$$N(x, u, \dots) = N^0 + \alpha \frac{\partial N}{\partial u} T_1 + \dots, \quad (6.15)$$

where we define $N^0 = N(x, u_0, \dots)$. Substituting (6.15) into (6.13) and retaining only terms linear in α we have

$$(L + \alpha N^0 + \lambda)u = 0. \quad (6.16)$$

Suppose that the unperturbed form ($\alpha = 0$) of Equation (6.16) has eigenvalues and normalized eigenfunctions given by

$$\lambda_0 = b_k, \quad (6.17)$$

$$u_0 = v_k(x), \quad (6.18)$$

respectively. Expanding the perturbed eigenfunctions $u(x)$ in terms of the unperturbed eigenfunctions $v_k(x)$ yields

$$u = \sum_k c_k v_k. \quad (6.19)$$

Substitution of (6.19) into (6.16) then gives

$$\sum_k (L + \alpha N^0 + \lambda) c_k v_k = 0. \quad (6.20)$$

Multiplying (6.20) by v_j and forming an inner product over the

1

1

fundamental domain we get

$$- \sum_k [(v_j, Lv_k) + \alpha(v_j, N^0 v_k)] c_k = \lambda c_j \delta_{jk} \quad (6.21)$$

or

$$- \sum_k (L_{jk} + \alpha N_{jk}^0) c_k = \lambda c_j, \quad (6.22)$$

where

$$L_{jk} = (v_j, Lv_k) \quad (6.23)$$

and

$$N_{jk}^0 = (v_j, N^0 v_k). \quad (6.24)$$

However, L has the diagonal representation

$$L_{jk} = -b_j \delta_{jk}, \quad (6.25)$$

so that (6.22) becomes

$$\sum_k (b_j \delta_{jk} - \alpha N_{jk}^0) c_k = \lambda c_j. \quad (6.26)$$

Thus diagonalization of the matrix $A_{jk} = b_j \delta_{jk} - \alpha N_{jk}^0$ will yield the perturbed eigenvalues λ . The matrix A referred to here is the same as that obtained by the operator method. It is the form of the differential equation that will generally determine which method should be adopted for the computation of the matrix elements.

A comparison with the standard perturbation theory can easily be made at this point. If, instead of multiplying Equation (6.20) by v_j , we multiply by v_k and form the inner product then (6.21) becomes

$$\sum_k [(v_k, Lv_k) + \alpha(v_k, N^O v_k) + \lambda] c_k = 0 \quad (6.27)$$

or

$$\sum_k [b_k - \alpha N_{kk}^O - \lambda] c_k = 0. \quad (6.28)$$

Thus

$$\lambda = b_k - \alpha N_{kk}^O, \quad (6.29)$$

which clearly defines the perturbed eigenvalues λ , for the standard perturbation method, as the diagonal elements of the matrix A.

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APPENDIX

APPENDIX

Computer Program

Listed below is a modification of a FORTRAN program originally developed by Green and Triffet for computing the eigenvalues and eigenvectors of a real matrix.⁹ Either symmetric or nonsymmetric matrices may be entered; once the matrix has been introduced, a check is made to determine whether it is symmetric or not, then the appropriate branch of the program is automatically selected.

The original program was written for a CDC 6400 computer, and some difficulties with accuracy arose when the program was run on an IBM 360 computer. To compensate for this, double precision calculations were introduced. Computation time was lengthened, but a 25X 25 matrix still only requires about 5 minutes.

A critical point in the program is the estimate of the largest eigenvalue. This appears to be even more important when multiple eigenvalues exist. An estimator technique, based on an iteration method for computing the magnitude of the largest eigenvalue, is built into the program. Before printout, a check is made of the largest eigenvalue by means of the estimator. If these values are not sufficiently close, the largest eigenvalue becomes the estimator and the procedure is repeated until convergence is reached - a process which may be accelerated, if necessary, by reducing the tolerance in FUNCTION DLEIG.

```

/JOB GO, TIME=10
/FTC

DOUBLE PRECISION SAVA(25,25), BIG1, ABIG1, AE
DOUBLE PRECISION TOL, A(50,25), B(25)
DOUBLE PRECISION AD, BC, AI, AE, BI, AJ, BA, BJ, AC, AK, BS, PK

111 JJ=9
    WRITE(6,433)
433  FORMAT(1H1)
    IBAD=0
    WRITE(6,200)
200  FORMAT(11X, 'ENTER THE ORDER N OF THE MATRIX IN 13 FORMAT. ')
    READ(JJ,201) N
201  FORMAT(13)
    WRITE(6,202) N
202  FORMAT(11X, 'N= ', I3)
    1  FORMAT(13, E16.8)
    NA=2*N
    DO 3 J=1, 25
    DO 2 I=1, 50
    2  A(I,J)=0.
    IZ=J+N
    3  A(IZ,J)=1.
    AC = 10.D-08
    WRITE(6,210)
210  FORMAT(11X, 'ENTER THE ELEMENTS OF THE MATRIX--FIRST ROW FIRST, ETC.
1  IN 5F16.8 FORMAT. FOR A MATRIX OF ORDER 6 THIS WOULD',/,11X, 'RECU
2  RE ENTRIES ON 8 LINES WITH EACH OF THE FIRST 7 LINES CONTAINING 5
3  NUMBERS PLACED IN THE PROPER FIELDS',/,11X, 'AND THE 8TH LINE CONT
4  AINING ONLY ONE NUMBER WHICH WOULD BE PLACED IN THE FIRST FIELD OF
5  THIS LAST LINE. ')
    READ(JJ,212)((A(I,J), J=1,N), I=1,N)
    DO 4 I=1,N
    DO 4 J=1,N
    4  SAVA(I,J)=A(I,J)
    WRITE(6,209)

```

```

209 FORMAT(11X,'IMMEDIATELY BELOW IS THE N BY N MATRIX ENTERED INTO TH
1E PROGRAM.')
DO 211 I=1,N
WRITE(6,1)I
DO 211 J=1,N,5
211 WRITE(6,212)A(I,J),A(I,J+1),A(I,J+2),A(I,J+3),A(I,J+4)
212 FORMAT(5F16.8)
TOL=10.**(-5)
DO 110 I=1,N
DO 110 J=1,N
IF(DABS(A(I,J)-A(J,I))-TOL)110,110,130
110 CONTINUE
300 IN=1
I=N
301 J=0
302 J=J+1
AI=A(I,I)
AJ=A(J,J)
AK=A(I,J)
AD=0.5*(AI+AJ)
AB=AI-AD
IF(DABS(AK)-DABS(AP)*AC) 308,308,303
303 IN=-1
BA=AB/AK
BS=DSQRT(1.D0 +BA*BA)
IF(BA)304,305,305
304 BS=-BS
305 BA=BA+BS
BS=1.D0/DSQRT(1.+BA*BA)
BC=BA*BS
DO 306 IA=1,NA
AI=A(IA,I)
A(IA,I)=AI*BC+A(IA,J)*BS
306 A(IA,J)=A(I,J)*BC-AI*PS
DO 307 IA=1,N

```

```

AI=A(I,IA)
A(I,IA)=BC*AI+BS*A(J,IA)
307 A(J,IA)=BC*A(J,IA)-BS*AI
308 I=I+1
IF(I-N)302,302,309
309 I=N-J
IF(I-1)310,310,301
310 IF(IN)300,311,311
311 I=N
DO 313 J=1,N
WRITE(6,314)J,A(J,J)
314 FORMAT(1H0,/,13,4X,'EIGENVALUE = ',E16.8)
L=2*N
M=N+1
WRITE(6,315)A(N,J),A(N+1,J),A(N+2,J),A(N+3,J),A(N+4,J)
315 FORMAT(12X,'VECTOR = ',5E16.8)
IF(N-5)313,313,316
316 M=N+6
DO 313 IA=N,L,5
WRITE(6,312)A(IA,J),A(IA+1,J),A(IA+2,J),A(IA+3,J),A(IA+4,J)
312 FORMAT(21X,5E16.8)
313 CONTINUE
GO TO 93
C   BRANCH BACK TO HERE WHEN ESTIMATOR IS BAD
120 CONTINUE
DO 122 I=1,N
DO 121 J=1,N
121 A(I,J)=SAV(I,J)
IZ=I+N
A(IZ,I)=1.
122 B(I)=0.
130 IB=N-2
21 DO 31 I=1,IB
JB=I+1
AI=A(JB,I)

```

```

IN=0
AB=0.
DO 23 J=JB,N
AJ=A(J,I)
B(J)=AJ
IF(DABS(AJ)-DABS(AI)*AC)23,23,22
22 IN=J
AB=AB+AJ*AJ
23 CONTINUE
IF(IN-JB)31,31,24
24 BA = DSOBT(AB)
IF(AI)25,26,26
25 BA=-BA
26 AB=AB+BA*AI
DO 28 IA=1,N
AK=BA*A(JB,IA)
DO 27 J=JB,N
27 AK=AK+B(J)*A(J,IA)
AK=AK/AB
A(JB,IA)=A(JB,IA)-BA*AK
DO 28 J=JB,N
28 A(J,IA)=A(J,IA)-B(J)*AK
DO 30 IA=1,NA
AK=BA*A(IA,JB)
DO 29 J=JB,N
29 AK=AK+A(IA,J)*B(J)
AK=AK/AB
A(IA,JB)=A(IA,JB)-BA*AK
DO 30 J=JB,N
30 A(IA,J)=A(IA,J)-AK*B(J)
31 CONTINUE
IF(IBAD) 324,32,324
32 AE=DLEIG(A,N)
WRITE(6,500) AE
500 FORMAT(' ESTIMATOR FROM DLEIG WAS',F12.6)

```

```

      IF(AE) 334,324,324
334  AE=-1.E50
      I=0
320  I=I+1
      IF(N-I)324,322,322
322  IF(AE-A(I,I))323,320,320
323  AE=A(I,I)
      GO TO 320
324  BC=0.25*AC
      ABIG1=AE
      AB=AE
42   JA=0
      IA=N-1
      IB=IA
43   JA=JA+1
      AI=A(1,1)-AB
      AJ=A(2,1)
      I=1
44   J=I+1
      BI=1.
      IN=-1
      IF(DABS(AJ)+BC*AI)47,47,45
45  BA = DSQRT(AI*AI+AJ*AJ)
      IN=1
      BI=AI/BA
      BJ=AJ/BA
      DO 46 JB=1,N
      AK=A(I,JB)
      A(I,JB)=BI*AK+BJ*AI(J,JB)
46  A(J,JB)=BI*AI(J,JB)-BJ*AK
47  AI=A(J,J)-AB*BI
      AJ=A(J+1,J)
      IF(IN)50,50,48
48  DO 49 JB=1,N
      AK=A(JB,I)

```

```

A(JB,I)=AK*RI+A(JB,J)*RJ
49 A(JB,J)=A(JB,J)*RI-AK*RJ
50 I=I+1
    IF(I-IA)44,44,51
51 IF(JA-N)52,52,61
52 AK=0.5*(A(IB+1,IB+1)-A(IR,IB))
    AJ=A(IB+1,IB)
    IF(DABS(AJ)-AC*DARS(AK)) 60,60,53
53 AI=A(IB,IB+1)
    AB=AK*AK+AI*AJ
    IF(AB)54,58,58
54 IF(DABS(AK)-AC*DABS(AJ)) 61,61,55
55 AI=0.5*(AI-AJ)
    BA = DSORT(AB +AI*AI)
    IF(AI+AJ)56,57,57
56 BA=-BA
57 AB=AJ*AK/(AJ+AI+BA)
    GO TO 59
58 AB = AK + DSORT(AB)
59 AB=A(IB,IB)+AB
    GO TO 43
60 IA=IR-1
61 JA=0
    IB=IB-1
    IF(IR)62,62,52
62 I=N
    IN=1
    AC=16.*AC
    DO 85 JB=2,N
    DO 84 J=JE,N
    I=J+1-JR
    BA=A(I,J)
    BI=A(J,J)-A(I,I)
    AI=B(J)
    B(J)=0.

```

```

IF(IN)72,72,71
71 IF(DABS(A(J,I))-AC*DABS(EI)) 73,73,84
72 IF(DABS(AI)-AC) 73,81,81
73 AI=BI*BA
  AK=BI*BI
  AJ=0.
  BK=0.
  IF(J-N)75,74,74
74 IF(I-1)80,80,78
75 BA=A(J+1,J+1)-A(J,J)
  AB=A(J+1,J)
  IF(DABS(AB)-DABS(BA))74,74,76
76 AI=AI-A(I,J+1)*AB
  AK=AK-A(J,J+1)*AB
  IF(I-1)80,80,77
77 AJ=AJ-A(I-1,J+1)*AB
78 BA=A(I,I)-A(I-1,I-1)
  AB=A(I,I-1)
  IF(DABS(AB)-DABS(EA)) 80,80,79
79 AI=AI-AB*A(I-1,J)
  BA=A(I-1,I)
  AJ=AJ+BI*A(I-1,J)-BA*A(I,J)
  AK=AK+AB*BA
  BK=2.*BI*AB
  BI=2.*BI*BI
  B(J)=AK*AJ+BI*AI
80 BI=AK*AK-BI*BK
  BA=AK*AI+BK*AJ
  B(J)=B(J)/BI
  AI=BA/BI
81 DO 82 IA=1,N
82 A(I,IA)=A(I,IA)-AI*A(J,IA)
  DO 83 IA=1,NA
83 A(IA,J)=A(IA,J)+AI*A(I,IA)
84 CONTINUE

```

```

C
C      COMPARE ESTIMATOR WITH ALGEBRAICALLY LARGEST EIGENVALUE.
C      IF ESTIMATOR IS BAD USE THE LARGEST CALCULATED EIGENVALUE
C      AS THE ESTIMATOR AND RETRY.
C
      BIG1=-1.E50
      DO 90 I=1,N
        90 BIG1=DMAX1(BIG1,A(I,I))
        IF(DABS(ABIG1)-TOL) 98,98,99
        98 RAT=BIG1*1000.
        GO TO 100
        99 RAT=(ABIG1-BIG1)/ABIG1
        100 IF(ABS(RAT)-.0001) 85,91,91
        91 IBAD=1
        AE=BIG1
        WRITE(6,411) BIG1
        411 FORMAT(7X'NEXT ESTIMATOR WAS'F12.6)
        GO TO 120
      85 IN=-1
      CALL NORM(A,N)
      911 FORMAT(5E16.8)
      97 DO 92 I=1,NA
        WRITE(6,1) I
        DO 92 J=1,N,5
          92 WRITE(6,911)A(I,J),A(I,J+1),A(I,J+2),A(I,J+3),A(I,J+4)
          WRITE(6,400)
          400 FORMAT(11X,'1. IMMEDIATELY ABOVE APPEARS A 2N BY N MATRIX.')
          WRITE(6,401)
          401 FORMAT(11X,'2. IF THE EIGENVALUES ARE REAL THEY APPEAR ON THE MAIN
            1 DIAGONAL OF THE FIRST N BY N MATRIX WITH ALL ELEMENTS',/,17X,'PFL
            2OW THE MAIN DIAGONAL NEGLIGIBLE.')
          WRITE(6,402)
          402 FORMAT(11X,'3. IF EIGENVALUES ARE COMPLEX THEY APPEAR AS TWO-DIMEN
            1SIONAL MATRICES ON THE DIAGONAL.')
          WRITE(6,403)

```

```
403 FORMAT(11X,'4. THE EIGENVECTORS ARE LISTED BY COLUMNS IN THE SECOND  
1D N BY N MATRIX. ONLY COMPONENT MAGNITUDES APPEAR FOR',/,17X,'COM  
2PLEX EIGENVECTORS.')
```

```
93 GO TO 111
```

```
END
```

```

C
C      DOUBLE PRECISION FUNCTION DLEIG(A,N)
C      TOL=1.D-06
C      DO 5 I=1,N
C      5 B(I) =1.D0

C      MULTIPLY B BY A AND ITRATE UNTIL RESULT CONVERGES.
C
C      RPREV =0.D0
C      NB=25
C      1 IR=0
C      IK=0
C      RBIG =0.D0
C      DO 15 J=1,N
C      IR = IR+1
C      JI = J-2*NB
C      IB=IK
C      R(IR)=0.D0
C      DO 10 I=1,N
C      JI = JI+2*NB
C      IB=IB+1
C      10 R(IR) =R(IR)+A(JI)*B(IB)
C      RBIG=DMAX1(DABS(RBIG),DABS(R(IR)))
C      IF(RBIG-DABS(R(IR)))15,11,15
C      11 RBIG=DSIGN(RBIG,R(IR))
C      15 CONTINUE
C      IF(DABS(RBIG-RPREV)-TOL)33,33,19
C      19 DO 20 J=1,N
C      20 B(J)=R(J)/DABS(RBIG)
C      RPREV =RBIG
C      GO TO 1
C      33 DLEIG = RBIG
C      RETURN
C      END

```

```
SUBROUTINE NORM(A,N)
DOUBLE PRECISION A(1),BEST
JUMP =50
I = N
IMAX =1250
1 BEST=DABS(A(I+1))
DO 5 J=2,N
  IPJ=I+J
  5 BEST = DMAX1(BEST,DABS(A(IPJ)))
  IF (BEST) 6,15,6
  6 DO 10 J=1,N
    IPJ=I+J
    10 A(IPJ) = A(IPJ)/BEST
    I = I +JUMP
    IF(I -IMAX) 1,15,15
  15 RETURN
END
```

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