JOURNAL OF COMPUTATIONAL PHYSICS 9, 53–74 (1972)

A New Method for Solving Eigenvalue Problems

E. WASSERSTROM*

Bell Telephone Laboratories, Murray Hill, New Jersey

Received March 30, 1971

A new method for calculating eigenvalues of ordinary differential operators is presented. After imbedding the given operator into a suitable one-parameter family of operators, the eigenvalue problem is reformulated as an initial-value problem. A numerical scheme for solving the initial-value problem is described and results of several examples are displayed. Both the self-adjoint and non-self-adjoint cases are treated. It is advantageous to supplement the above method by an efficient iterative scheme, and an example of the latter is therefore shown. Finally, we briefly discuss the advantage and drawbacks of our method.

I. INTRODUCTION

Classical numerical methods for solving boundary-value problems, and, in particular, eigenvalue problems, are rather cumbersome [1, 2]. On the other hand, computers are particularly suitable for solving large systems of (linear or nonlinear) first-order ordinary differential equations with given initial values. In this paper we shall describe a new method, by which the "simple" eigenvalue problem is reformulated as a "complicated" initial-value problem, which is, however, more adaptable to numerical solutions. In fact, this method is a special case of the continuation method [3], which has been applied by us also to the problem of finding roots of polynomials [4] and to boundary value problems [5].

The basic idea of the continuation method is rather simple: instead of the given problem one solves a similar but simpler ("base") problem. Then this solution of the base is "continued" until the original problem is reached. The continuation method has been employed extensively over the last century in theoretical proofs of existence proofs of linear and nonlinear problems. A summary and some historical remarks can be found in the survey of Ficken [6], and the more recent works of Meyer [7] and Laasonen [8]. The merit of this method is that it naturally lends itself to the reformulation of problems as initial-value ones.

* Mr. Wasserstrom has returned to the Technion–Israel Institute of Technology, Haifa, Israel.

Davidenko [9] was apparently the first who implicitly applied the continuation method to the numerical evaluation of zeros of a system of equations; subsequent work can be found in Refs. [4, 10–12]. A method which is very close to the continuation method was invented by Bellman, Kalaba, and their coworkers. They called it "invariant imbedding" and applied it successfully to a wide variety of transport problems [13, 14] integral equations [15, 16] and others. Shoemaker [17], and more recently Scott *et al* [18], showed how the invariant imbedding method can be applied to the calculation of eigenvalues. In fact, the idea of transforming a boundary-value problem into an initial-value one goes back, at least, to Blasius' classical solution of the boundary layer [19]. Extension of his approach by considering different linear (and nonlinear) transformations of the dependent and independent variables was carried out by several investigators [20–22]. The continuation method is capable of treating a much wider range of problems by transforming the operator itself.

In the next section we formulate the continuation method for finding eigenvalues of self-adjoint ordinary differential operators. In Section III we treat the important special case of a Sturm–Liouville system, and in Section IV details of two numerical examples are given. In Section V, the method is extended to nonself-adjoint operators. In Section VI an iterative scheme is sketched, and finally in Section VII we make some concluding remarks.

II. Formulation of the Method

Consider the following eigenvalue problem [23]

$$L_1 y_1 = \lambda_1 y_1 , \tag{2.1}$$

where

$$L_1 = \sum_{n=0}^{N} a_{(n)}^{(1)}(x) \frac{d^n}{dx^n} , \tag{2.2}$$

where $a_n^{(1)}(x)$ are functions of class C^n on the closed interval $a \leqslant x \leqslant b$ and $a_N^{(1)}(x) \neq 0$ on $[a, b]$. The eigenfunctions $y_1(x)$ should also satisfy the homogeneous boundary conditions

$$U_1^{(j)} y_1 \equiv \sum_{k=1}^{N} \left[b_{jk} \frac{d^{k-1} y_1}{dx^{k-1}} (a) + c_{jk} \frac{d^{k-1} y_1}{dx^{k-1}} (b) \right] = 0, \qquad j = 1, 2, \ldots, N, \tag{2.3}$$

where the b_{jk} and c_{jk} are constants. Let us also assume that the problem (2.1–2.3) is self-adjoint. It is known [23] that the eigenvalues λ_1 are real and constitute an at

most enumerable set with no finite cluster point; in addition, it will be assumed that they are distinct. In what follows we shall show how to compute these eigenvalues and the corresponding eigenfunctions by the continuation method.

Let us imbed L_1 into a one-parameter family of operators $L(t)$ as follows

$$L(t)\, y(t, x) = \lambda(t)\, y(t, x), \tag{2.4}$$

where we have emphasized the t-dependence of the family L which is defined by

$$L(t) = \sum_{n=0}^{N} a_n(t, x) \frac{\partial^n}{\partial x^n}. \tag{2.5}$$

The functions $a_n(t, x)$ have continuous t derivatives, and for $t \in [0, 1]$ have the properties defined after Eq. (2.2). The eigenfunctions $y(t, x)$ should satisfy the boundary conditions

$$U^{(j)}(t)\, y \equiv \sum_{k=1}^{N} \left[b_{jk} \frac{\partial^{k-1} y}{\partial x^{k-1}}(t, a) + c_{jk} \frac{\partial^{k-1} y}{\partial x^{k-1}}(t, b) \right] = 0, \qquad j = 1, 2, \ldots, N, \tag{2.6}$$

for $0 \leqslant t \leqslant 1$.

In addition to the above requirements, the functions $a_n(t, x)$ are chosen so that

(i) At $t = 0$, the eigenvalue problem

$$\begin{aligned} L(0)\, y(0, x) &= \lambda(0)\, y(0, x), \\ U^{(j)}(0)\, y &= 0, \end{aligned} \tag{2.7}$$

can somehow be solved. The corresponding eigenvalues

$$\lambda_0 = \lambda(0) \tag{2.8}$$

will be referred to as the base.

(ii) At $t = 1$,

$$a_n(1, x) = a_n^{(1)}(x). \tag{2.9}$$

See Eq. (2.2).

(iii) For $0 \leqslant t \leqslant 1$ the problem (2.4–2.6) is self-adjoint with distinct eigenvalues.

In order to formulate an initial-value problem for the eigenvalues $\lambda(t)$ we differentiate Eq. (2.4) with respect to t and get

$$\dot{L}y + L\dot{y} = \dot{\lambda} y + \lambda \dot{y}, \tag{2.10}$$

where dots denote t-derivatives so that

$$\dot{L} = \sum_{n=0}^{N} \dot{a}_n(t, x) \frac{\partial^n}{\partial x^n}. \tag{2.11}$$

Differentiating Eq. (2.6) with respect to t, we obtain

$$U^{(i)}(t)\,\dot{y} = 0. \tag{2.12}$$

Next, we take the inner product of Eq. (2.10) with y,

$$(\dot{L}y, y) + (L\dot{y}, y) = \dot{\lambda}(y, y) + \lambda(\dot{y}, y), \tag{2.13}$$

where the inner product of two functions $f(t, x)$ and $g(t, x)$ is defined by

$$(f, g) \equiv w_1(t) = \int_a^b f(t, \xi)\, \bar{g}(t, \xi)\, d\xi, \tag{2.14}$$

where the bar denotes the complex conjugate. Since L is self-adjoint and $\dot{y}$ satisfies the boundary condition (2.12), the second term on the left of Eq. (2.13) can be written as

$$(L\dot{y}, y) = (\dot{y}, Ly) = (\dot{y}, \lambda y) = \lambda(\dot{y}, y), \tag{2.15}$$

where in the last equality we have used the property that the eigenvalues of self-adjoint operators are real. Hence this term cancels out the last term on the right-hand side of Eq. (2.13), and we obtain

$$\dot{\lambda}^{(i)}(t) = (\dot{L}y^{(i)}, y^{(i)})/(y^{(i)}, y^{(i)}), \qquad i = 1, 2,..., \tag{2.16}$$

where the superscript i orders the eigenvalues and the corresponding eigenfunctions.

Equations (2.16) represent a system of uncoupled, first-order, nonlinear ordinary differential equations. The initial values of this system are given by

$$\lambda^{(i)}(0) = \lambda_0^{(i)}, \qquad i = 1, 2,..., \tag{2.17}$$

where $\lambda_0^{(i)}$ is our base, Eq. (2.8). If we could integrate Eqs. (2.16, 2.17) from $t = 0$ until $t = 1$ we would get

$$\lambda^{(i)}(1) = \lambda_1^{(i)}, \qquad i = 1, 2,..., \tag{2.18}$$

which, because of our choice of (2.9) is the solution of our original problem, Eqs. (2.1–2.3).

The numerical integration of Eqs. (2.16, 2.17) is carried out in two interwoven stages, which are arranged as nested loops [24] in the computer program. In the first stage, or the inner loop, we evaluate the right hand side of Eq. (2.16) assuming that t and $\lambda^{(i)}(t)$ are known from the outer loop. This is done by solving the following initial-value problem [23]

$$\begin{aligned} L(t)\,\phi_j &= \lambda^{(i)}\phi_j\,, \qquad j = 1, 2,..., N, \\ [\partial^{k-1}\phi_j(a)]/\partial x^{k-1} &= \delta_{jk}\,, \qquad j, k = 1, 2,..., N, \end{aligned} \tag{2.19}$$

where for simplicity $\phi_j^{(i)}(t, \lambda^{(i)}, x)$ is written as $\phi_j(x)$. The corresponding eigenfunction

$$y^{(i)} = \sum_{j=1}^{N} \alpha_j \phi_j\,, \tag{2.20}$$

is found by solving the linear (inhomogeneous) system of $N - 1$ equations

$$\sum_{j=1}^{N} \alpha_j U^{(k)}(t)\,\phi_j = 0, \qquad k = 1, 2,..., N - 1, \tag{2.21}$$

for the constants α_j, [see Eq. (2.6)]. Since the eigenvalues were assumed to be distinct, the rank of the matrix of (2.21) is $N - 1$ [23] and therefore the solutions $\alpha_j, j = 1, 2,..., N$, are determined up to an arbitrary multiplicative factor. The last equation corresponding to $k = N$ serves as a compatibility equation. If we insert the constants α_j into it we get

$$\sum_{j=1}^{N} \alpha_j U^{(N)}(t)\,\phi_j = \epsilon_N\,, \tag{2.22}$$

where the small ϵ_N is a measure of the error introduced by the truncation and round-off errors. Knowing $y^{(i)}$ we can evaluate the right-hand side of Eq. (2.16).

We are now ready for the second stage, which is the outer loop in the numerical program. In the previous stage we have computed $G(t, \lambda^{(i)})$ where

$$d\lambda^{(i)}/dt = G(t, \lambda^{(i)}) \tag{2.23}$$

[see Eq. (2.16)]. The numerical integration of the last equation with initial values (2.17) produces the desired eigenvalues λ_1 at $t = 1$ [see Eq. (2.18)]. It is a nice feature of this method that one can pick out any specific eigenvalue, say the 17th, and determine it independently of the others. Further details about this scheme will accompany the example which is described in the next section.

In order to insure the existence and uniqueness of the solution $\lambda^{(i)}(t)$ of Eqs. (2.23, 2.17), the function $G(t, \lambda^{(i)})$ should be continuous in t and satisfy a

Lipschitz condition in $\lambda^{(i)}$ in a domain containing the trajectory $\lambda^{(i)}(t)$. These conditions are met in our case: G is continuous in t since the functions $a_n(t, x)$ were required to possess continuous t-derivatives, see Eqs. (2.16) and (2.11). To show that G satisfies a Lipschitz condition with respect to $\lambda^{(i)}$ we have to use the theorem [25] on the continuous dependence of the solution ϕ_j of Eqs. (2.19) on the parameter $\lambda^{(i)}$, and the continuous dependence of the coefficients α_j on $\lambda^{(i)}$ in Eq. (2.21). Hence the integration of Eqs. (2.16, 2.17) from $t = 0$ to $t = 1$ is equivalent to solving the original problem (2.1–2.3).

III. Sturm–Liouville Problem

As an example of the application of the method described in the previous section, let us consider here the Sturm–Liouville eigenvalue problem

$$L_1 y_1 = -(p_1(x)\, y_1'(x))' + q_1(x)\, y_1(x) = \lambda_1 r_1(x)\, y_1(x), \tag{3.1}$$

where primes denote differentiation with respect to x. Here $p_1(x) > 0$, $r_1(x) > 0$ and $q_1(x) \geqslant 0$, while $p_1'(x)$ and $r_1(x)$ are continuous on [0, 1]. The eigenfunctions $y_1(x)$ satisfy the homogeneous boundary conditions

$$b_1 y_1(0) - b_2 y_1'(0) = 0, \tag{3.2a}$$

and

$$c_1 y_1(1) + c_2 y_1'(1) = 0, \tag{3.2b}$$

where the b's and c's are nonnegative constants, and at least one of each pair does not vanish. It is known that Eqs. (3.1, 3.2) determine an infinite sequence of nonnegative distinct eigenvalues, and in what follows we shall show how to find them by the continuation method described in Section II.

Corresponding to Eqs. (2.4–2.6) we have here the imbedding

$$L(t)\, y(t, x) = -(p(t, x)\, y')' + q(t, x)\, y = \lambda(t)\, r(t, x)\, y, \tag{3.3}$$

with boundary conditions

$$b_1 y(t, 0) - b_2 y'(t, 0) = 0, \tag{3.4a}$$

$$c_1 y(t, 1) + c_2 y'(t, 1) = 0, \tag{3.4b}$$

for $t \in [0, 1]$. Because of the factor $r(t, x)$ on the right hand side of Eq. (3.3), the differential Eq. (2.16) has here a slightly different form, i.e.,

$$\dot{\lambda}^{(i)}(t) = ((\dot{L} - \lambda^{(i)}\dot{r})\, y^{(i)}, y^{(i)})/(r y^{(i)}, y^{(i)}), \qquad i = 1, 2, \ldots. \tag{3.5}$$

An obvious choice for the functions p, q and r which satisfy conditions (i–iii) of Section II is

$$\begin{aligned} p(t, x) &= 1 - t + p_1(x)\, t, \\ q(t, x) &= q_1(x)\, t, \\ r(t, x) &= 1 - t + r_1(x)\, t. \end{aligned} \tag{3.6}$$

With this choice, Eq. (3.3) becomes at $t = 0$

$$y_0'' + \lambda_0 y_0 = 0, \tag{3.7}$$

where $y_0 \equiv y(0, x)$. For given b's and c's it is a simple matter to find the eigenvalues and eigenfunctions of this equation which satisfy boundary conditions (3.4) at $t = 0$. For example, if

$$b_2 = c_2 = 0, \tag{3.8}$$

we get our base

$$\lambda_0^{(i)} = \lambda^{(i)}(0) = i^2\pi^2, \qquad i = 1, 2,..., \tag{3.9}$$

and the corresponding eigenfunctions

$$y_0^{(i)} = \sin(i\pi x), \qquad i = 1, 2,... . \tag{3.10}$$

The solution of Eqs. (3.1, 3.2) is found by integrating Eqs. (3.5, 3.9) from $t = 0$ until $t = 1$.

In order to evaluate the right hand side of Eq. (3.5) it is convenient to define the two-variable function, see Eq. (2.14),

$$w(t, x) = \int_0^x f(t, \xi)\, g(t, \xi)\, d\xi, \tag{3.11}$$

so that the inner product of the two real functions f and g is

$$w(t, 1) = w_1(t) = (f, g), \tag{3.12}$$

and

$$w'(t, x) = f(t, x)\, g(t, x), \tag{3.13}$$

where the prime denotes partial differentiation with respect to x. Similarly, we define

$$u'(t, x) = y(\dot{L} - \lambda \dot{r})\, y, \tag{3.14}$$

and

$$v'(t, x) = r y^2, \tag{3.15}$$

so that Eq. (5) can be written as

$$\lambda = \frac{u(t, 1)}{v(t, 1)}. \tag{3.16}$$

The numerical solution is executed as a nested loop. In the inner loop t and $\lambda(t)$ are known (from the outer loop) and we wish to compute the right hand side of Eq. (3.16). In order to do this the second-order differential Eq. (3.3) is written as a pair of first-order differential equations

$$y' = z, \tag{3.17}$$

$$z' = y'' = p^{-1}(-p'z + qy - \lambda ry). \tag{3.18}$$

The other two equations are furnished by Eqs. (3.14, 3.15). Substituting Eqs. (3.3) and (3.6) into Eqs. (3.14, 3.15) we get after a few manipulations

$$u' = (1 - p_1)\, z'y - p_1'zy + q_1 y^2 - \lambda(r_1 - 1)\, y^2, \tag{3.19}$$

where z' is given by Eq. (3.18), and

$$v' = ry^2. \tag{3.20}$$

The initial values of Eqs. (3.17–3.20), for the special case with Eq. (3.8), are

$$y(t, 0) = 0, \tag{3.21}$$

$$z(t, 0) = 1, \tag{3.22}$$

$$u(t, 0) = 0, \tag{3.23}$$

and

$$v(t, 0) = 0. \tag{3.24}$$

Condition (3.22) is arbitrary, since the eigenfunctions are determined only up to an arbitrary multiplicative factor.

The initial-value problem (3.17–3.24) is in the standard form suitable for numerical integration by available programs, e.g., Runge–Kutta method. The integration is carried out until $x = 1$, and there we compute

$$G(t, \lambda) = u(t, 1)/v(t, 1). \tag{3.25}$$

We are now ready for the second stage which is the outer loop in the computer program. Comparing Eqs. (3.16) and (3.25) we see that

$$\lambda^{(i)}(t) = G(t, \lambda^{(i)}), \qquad i = 1, 2, \ldots, \tag{3.26}$$

where we have emphasized that this is a system of identical uncoupled equations but with different initial values. Equations (3.26, 3.9) are again an initial-value problem and can be easily integrated numerically. The t-integration is carried out until $t = 1$, and the final values

$$\lambda_1^{(i)} = \lambda^{(i)}(1) \tag{3.27}$$

are the solution of the original problem (3.1), since from Eqs. (3.6) we see that

$$L(1) = L_1 . \tag{3.28}$$

Similarly, the eigenfunctions of Eq. (3.1) are given by

$$y_1^{(i)}(x) = y^{(i)}(1, x). \tag{3.29}$$

This solves our problem.

The proof for the existence and uniqueness of the solution of Eqs. (3.26, 3.9) was sketched in the previous section. In particular, we note that for $t \in [0, 1]$ L is a Sturm–Liouville operator whose eigenvalues are distinct, so that the trajectories $\lambda^{(i)}t$ do not cross and the derivatives $\dot{\lambda}^{(i)}(t)$ are well defined. In contrast to the initial-value problems (3.17–3.24; 3.26, 3.9), the original problem is not continuous in λ_1 : if λ_1 is only infinitesimally different from an eigenvalue, the only solution of Eqs. (3.1, 3.2) is the trivial one $y_1 = 0$. In our solution the condition (3.4b) is not strictly satisfied [see also Eq. (2.22)], and in the special case (3.8) the difference of $y(t, 1)$ from zero is a measure of the error introduced by the numerical computations.

It should be stressed that it is essential for our method that the numerical integration of the outer loop (3.26, 3.9) is performed discretely and not continuously as is done, for example, by analog computers. Hence the interval $0 \leqslant t \leqslant 1$ is divided into a *finite* number of steps $0 < t_1 < t_2 < \cdots < t_j < \cdots < 1$, and at each step the function $G(t_j , \lambda^{(i)}(t_j))$ is evaluated by integrating the inner loop (3.17–3.24). This latter integration can be done in principle also by an analog computer. See also Section VII.

IV. Numerical Examples

The continuation method as formulated in the previous sections is not restricted to regular equations. It was applied, for example, to finding the eigenvalues and eigenfunctions of the (singular) Bessel equation

$$-(xy_1')' = \lambda_1 x y_1 , \tag{4.1}$$

with the boundary conditions

$$y_1'(0) = 0 \qquad \text{and} \quad y_1(1) = 0. \tag{4.2}$$

The singularity at $x = 0$ is easily removed by L'Hospital rule.

A program was written to solve this problem on a GE-635 computer using an available integrating subroutine [26]. The errors in the computations are controlled by a convergence criterion, the standard error δ, which is built in the integrating subroutine. (The standard error is defined as $| \sigma/y_M |$, where σ is the difference between two successive approximations, and y_M is the largest absolute value attained so far in the integration). The first five eigenvalues and eigenfunctions were computed, with standard errors for the x and t integrations of $\delta_x = \delta_t = .01$. Four eigenvalues were correct to five significant digits, whereas the eigenvalue corresponding to $i = 3$ was correct to only three significant digits. The computations took relatively long time—two minutes. In Fig. 1 we show the trajectories $[\lambda^{(i)}(t)]^{1/2}$ for $0 \leqslant t \leqslant 1$ for these five eigenvalues. In Figs. 2 and 3 we show the t-development of the first and third eigenfunctions $y^{(i)}(t, x)$ for $t = 0, .2, .5, .8,$ and 1.

One of the advantages of the present method is its flexibility. The program which was written can handle the general Sturm–Liouville problem, Eqs. (3.1, 3.2); all that one has to do in order to solve a specific problem is to specify the functions p_1, q_1 and r_1, the constants b_1, b_2, c_1 and c_2, and the standard errors δ_x and δ_t.

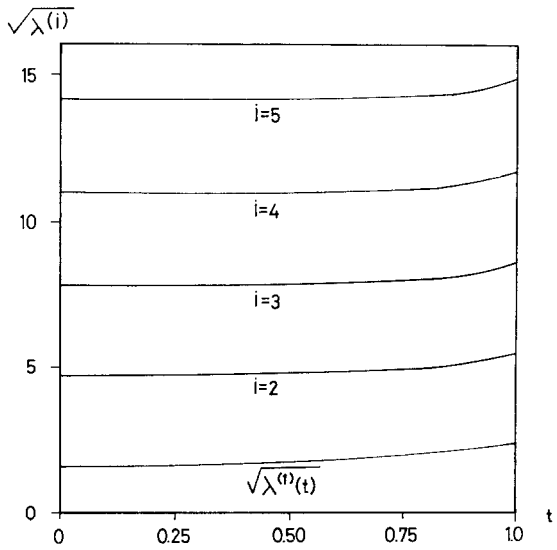

FIG. 1. Trajectories of the first five eigenvalues of the Bessel Eq. (4.1, 4.2).

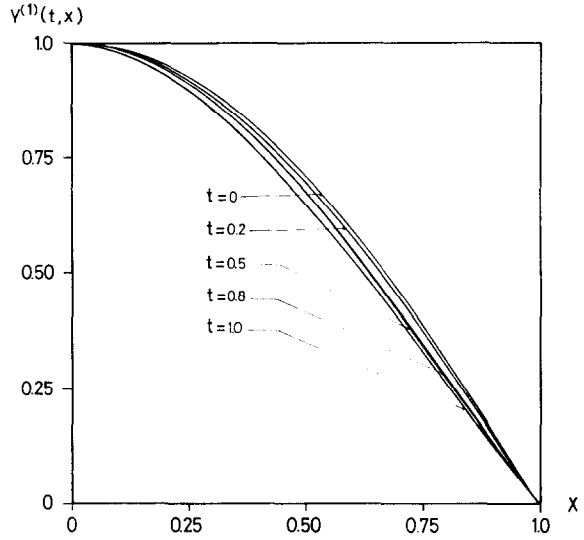

FIG. 2. Development of the first eigenfunction of the Bessel equation.

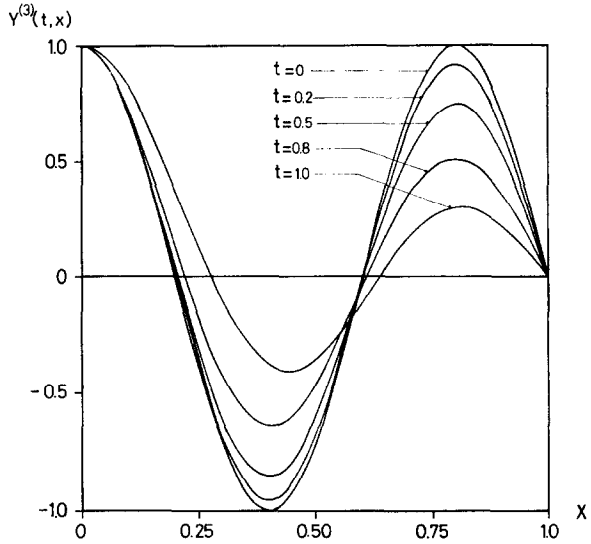

FIG. 3. Development of the third eigenfunction of the Bessel equation.

As a second example, we solved the following eigenvalue problem which arises in heat transfer theory [27]

$$-(xy_1')' = 4\lambda_1 x(1 - x^2)\, y_1 , \tag{4.3}$$

with boundary conditions

$$y_1'(0) = 0, \qquad y_1'(1) = 0. \tag{4.4}$$

This was done by changing only two (!) cards in the program which solved the previous problem, Eqs. (4.1, 4.2). The first ten eigenvalues and eigenfunctions were computed with standard errors $\delta_x = \delta_t = .001$. Again all eigenvalues except for the third were correct to at least five significant digits. The computations took six minutes on the GE-635. In Fig. 4 we show the trajectories $(\lambda^{(i)}(t))^{1/2}$ for $0 \leqslant t \leqslant 1$ for the first five eigenvalues. Ways to reduce the computation time are discussed in Section VI.

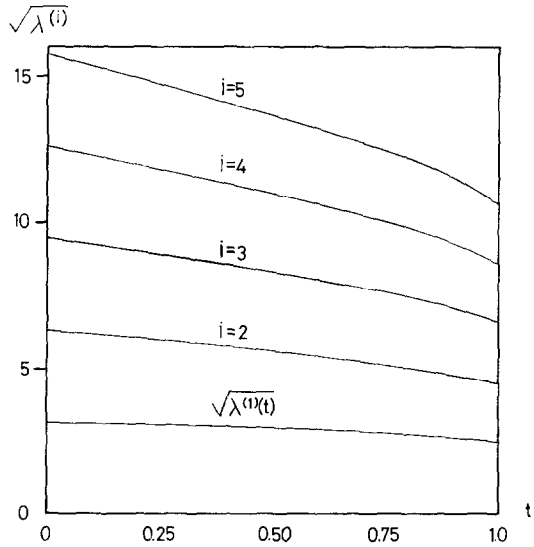

FIG. 4. Trajectories of the first five eigenvalues of Eqs. (4.3, 4.4).

V. NONSELF-ADJOINT PROBLEMS

We turn again to the eigenvalue problem (2.1–2.3) except that now we do not assume that it is self-adjoint. We proceed as before and imbed this problem according to Eqs. (2.4–2.6). The functions $a_n(t, x)$ should satisfy requirements (i) and (ii),

[Eqs. (2.7–2.9)] but not requirement (iii). In order to solve this problem by the continuation method it is necessary to consider also the adjoint problem [28]

$$L^{\dagger}(t)\, z(t, x) = \mu(t)\, z(t, x), \tag{5.1}$$

where $L^{\dagger}$ is the adjoint of L and is given by

$$L^{\dagger}(t) = (-1)^N (\partial^N/\partial x^N)\, \bar{a}_N + (-1)^{N-1} (\partial^{N-1}/\partial x^{N-1})\, \bar{a}_{N-1} + \cdots + \bar{a}_0\,, \tag{5.2}$$

where bars denote complex conjugates. The adjoint boundary conditions

$$U^{\dagger(j)}(t)\, z(t, x) = 0, \qquad j = 1, 2,..., N, \tag{5.3}$$

are determined so that for $t \in [0, 1]$

$$(Ly, z) = (y, L^{\dagger}z), \tag{5.4}$$

where the inner product was defined in Eq. (2.14).

If all the poles of the Green's function of the problem (2.4–2.6) for $t \in [0.1]$ are simple, then the eigenfunctions of this problem $y^{(i)}$ and those of the adjoint problem (5.1–5.3) $z^{(j)}$ satisfy a biorthogonal relation [28]

$$(y^{(i)}, z^{(j)}) = \delta_{ij}\,. \tag{5.5}$$

If $y^{(i)}$ has an eigenvalue $\lambda^{(i)}$, then the corresponding eigenfunction $z^{(i)}$ has an eigenvalue $\bar{\lambda}^{(i)}$, i.e.,

$$\mu^{(i)}(t) = \bar{\lambda}^{(i)}(t). \tag{5.6}$$

In order to derive the initial-value problem for $\lambda(t)$, we differentiate Eqs. (2.4, 2.6) with respect to t as before and obtain Eqs. (2.10–2.12). Here we diverge from the previous development. We take the inner product of Eq. (2.10) with z and get

$$(\dot{L}y, z) + (L\dot{y}, z) = \dot{\lambda}(y, z) + \lambda(\dot{y}, z). \tag{5.7}$$

The second terms on the left hand side of Eq. (5.7) can be written as

$$(L\dot{y}, z) = (\dot{y}, L^{\dagger}z) = (\dot{y}, \mu z) = \bar{\mu}(\dot{y}, z). \tag{5.8}$$

Noting Eq. (5.6) we see that for corresponding eigenfunctions this term cancels out the last term on the right hand side of Eq. (5.7) and we obtain

$$\dot{\lambda}^{(i)}(t) = (\dot{L}y^{(i)}, z^{(i)})/(y^{(i)}, z^{(i)}), \qquad i = 1, 2,\ldots\,. \tag{5.9}$$

If we could integrate Eqs. (5.9) with initial values (2.17) from $t = 0$ until $t = 1$, we would get

$$\lambda^{(i)}(1) = \lambda_1^{(i)}, \qquad i = 1, 2,..., \tag{5.10}$$

which because of our choice of (2.9) is the solution of our original problem [Eqs. (2.1–2.3)].

In order to demonstrate our method let us consider the simple nonself-adjoint problem

$$L_1 y_1 = -\left(\frac{d^2}{dx^2} + a_1 \frac{d}{dx} + b_1\right) y_1 = \lambda_1 y_1 , \tag{5.11}$$

where $a_1 \neq 0$ and b_1 are given real constants, and where the eigenfunctions satisfy the boundary conditions

$$y_1'(0) = y_1'(1) = 0. \tag{5.12}$$

An appropriate imbedding is

$$L(t)\, y(t, x) = -\left(\frac{\partial^2}{\partial x^2} + a_1 t \frac{\partial}{\partial x} + b_1 t\right) y(t, x) = \lambda(t)\, y(t, x), \tag{5.13}$$

with boundary conditions

$$y'(t, 0) = y'(t, 1) = 0. \tag{5.14}$$

It is easy to show that the adjoint problem is

$$L^{\dagger}(t)\, z(t, x) = -\left(\frac{\partial^2}{\partial x^2} - a_1 t \frac{\partial}{\partial x} + b_1 t\right) z(t, x) = \mu(t)\, z(t, x), \tag{5.15}$$

with boundary conditions

$$a_1 t z(t, 0) - z'(t, 0) = 0, \tag{5.16a}$$

$$a_1 t z(t, 1) - z'(t, 1) = 0. \tag{5.16b}$$

The base, i.e., the solution of Eqs. (5.13, 5.14) at $t = 0$ is

$$\lambda_0^{(i)} = \lambda^{(i)}(0) = (i\pi)^2, \qquad i = 1, 2,..., \tag{5.17}$$

and the corresponding eigenfunctions

$$y_0^{(i)}(x) = y^{(i)}(0, x) = \cos(i\pi x), \qquad i = 1, 2,... . \tag{5.18}$$

In order to formulate the initial-value problem for this example, we substitute Eq. (5.13) into (5.9) and get

$$\frac{d\lambda^{(i)}}{dt} = -\frac{\int_0^1 (a_1 y^{(i)\prime} + b_1 y^{(i)})\, z^{(i)}\, dx}{\int_0^1 y^{(i)} z^{(i)}\, dx} \equiv \frac{u^{(i)}(t, 1)}{v^{(i)}(t, 1)}, \qquad i = 1, 2,..., \tag{5.19}$$

where

$$u'(t, x) = -(a_1 y' + b_1 y)\, z, \tag{5.20}$$

$$v'(t, x) = yz, \tag{5.21}$$

and for conciseness we have deleted the superscript i. The numerical procedure proceeds as in the self-adjoint case. In the inner loop, t and λ are assumed to be known from the outer loop, and we evaluate the right hand side of Eq. (5.19) by solving the following initial-value problem (in addition to Eqs. (5.20, 5.21)):

$$y' = p, \tag{5.22}$$

$$p' = y'' = -a_1 tp - b_1 ty - \lambda y, \tag{5.23}$$

$$z' = q, \tag{5.24}$$

$$q' = z'' = a_1 tq - b_1 tz - \lambda z. \tag{5.25}$$

The initial values for Eqs. (5.20–5.25) are

$$y(t, 0) = 1, \tag{5.26}$$

$$p(t, 0) = 0, \tag{5.27}$$

$$z(t, 0) = 1, \tag{5.28}$$

$$q(t, 0) = a_1 t, \tag{5.29}$$

$$u(t, 0) = 0, \tag{5.30}$$

$$v(t, 0) = 0. \tag{5.31}$$

Conditions (5.26) and (5.28) are arbitrary, since the eigenfunctions are determined only up to an arbitrary factor. Note that since Eq. (5.14) is independent of t, $\dot{y}$ also satisfies this equation as was required for the derivation of Eq. (5.19) [see also Eq. (2.12)]. On the other hand, condition (5.16) explicitly depends on t and therefore $\dot{z}$ does not (and does not have to) satisfy this equation.

The system (5.20–5.31) is integrated numerically until $x = 1$, and there we compute

$$G(t, \lambda) = u(t, 1)/v(t, 1). \tag{5.32}$$

The outer loop consists of the integration of Eq. (5.19) with initial values given by Eq. (5.17). The final values of the integration

$$\lambda^{(i)}(1) = \lambda_1^{(i)} \tag{5.33}$$

are the solution of the original problem (5.11, 5.12) since $L(1) = L_1$.

A program was written to solve this problem on the GE-635 using an available integrating subroutine [26]. As a numerical example, we chose $a_1 = 4$ $b_1 = -5$. In Fig. 5 we show the trajectories $(\lambda^{(i)}(t))^{1/2}$ for $0 \leqslant t \leqslant 1$ and $i = 1$–5, (because of an oversight, the case $i = 0$ was not computed). In Fig. 6 we show the development of $y^{(2)}(t, x)$ for $t = 0, .25, .5, .75$, and 1.

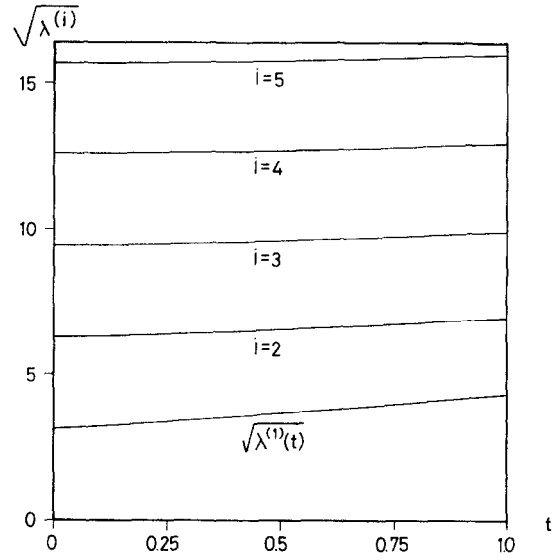

FIG. 5. Trajectories of the eigenvalues $i = 1$–5 of the nonself-adjoint Eqs. (5.11, 5.12) with $a_1 = 4$ and $b_1 = -5$.

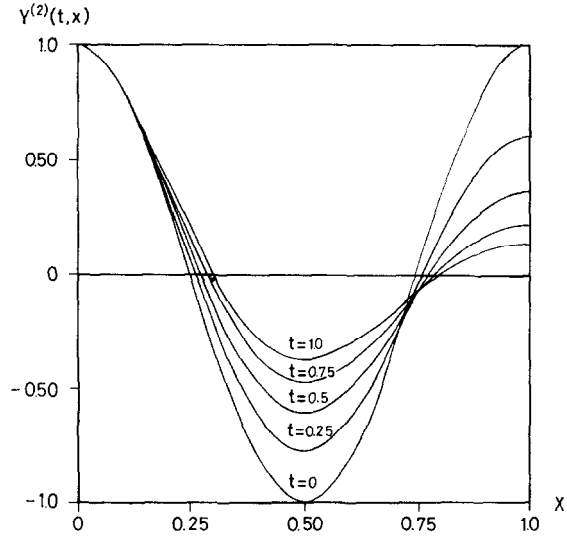

FIG. 6. Development of the second eigenfunction of the nonself-adjoint problem.

VI. An Iterative Scheme

The main drawback of the continuation method presented above is that it is rather slow. The reason for this is clear; in effect, one has to solve accurately many intermediate problems for $0 < t < 1$, whose solution is usually not of interest, in order to reach the solution of the original problem at $t = 1$. Therefore if one seeks highly accurate values for the eigenvalues, it is worth while to proceed as follows. First compute with the continuation method a rather crude result by choosing a large integration step size. Then use this result as a starting approximation in some efficient iterative method. If this starting value is in the "domain of attraction" [29] of the desired solution, then the iterative scheme will converge.

There exist many iterative schemes for eigenvalue problems. A simple and efficient method à la Regula Falsi is presented in [27]. Here we shall sketch a scheme which is a variant of the Rayleigh–Ritz method and which is easily incorporated in the program described in the previous sections. Taking the inner product of Eq. (2.1) with y_1 we obtain

$$\lambda_1^{(i)} = (L_1 y_1^{(i)}, y_1^{(i)})/(y_1^{(i)}, y_1^{(i)}), \tag{6.1}$$

where L_1 is not necessarily self-adjoint.

Let us expand y_1 and λ_1 as follows:

$$y_1(x) = \eta^{(0)}(x) + \eta^{(1)}(x) + \cdots, \tag{6.2}$$

$$\lambda_1 = \sigma^{(0)} + \sigma^{(1)} + \cdots, \tag{6.3}$$

where $\| \eta^{(1)}(x)\| \ll \| \eta^{(0)}(x)\|$ and $| \sigma^{(1)} | \ll | \sigma^{(0)} |$. Substituting the last equations in Eq. (6.1) we obtain after several manipulations the following expression for the first-order correction to the eigenvalue

$$\sigma^{(1)} = (\eta^{(0)}, \eta^{(0)})^{-1} [(L_1\eta^{(1)}, \eta^{(0)}) - \sigma^{(0)}(\eta^{(1)}, \eta^{(0)})]. \tag{6.4}$$

Expansions like (6.2, 6.3) and results similar to Eq. (6.4) were already created by Rayleigh and Schrodinger and were rigorously studied by Rellich [30]. In our scheme we take, as initial approximation,

$$\eta^{(0)}(x) = y(1, x), \tag{6.5}$$

and

$$\sigma^{(0)} = \lambda(1), \tag{6.6}$$

where the right hand sides of these equations are obtained from the computations of the continuation method, which because of truncation and round-off errors do not yield the exact solutions of Eqs. (2.1–2.3).

For simplicity, let us restrict ourselves from now on to the Sturm–Liouville problem (3.1, 3.2). A simple choise for $\eta^{(1)}$ is

$$\eta^{(1)}(x) = kx^2, \tag{6.7}$$

where the coefficient k is determined so that $\eta^{(0)} + \eta^{(1)}$ satisfy boundary conditions (3.2). From Eqs. (3.21, 3.22) we see that $\eta^{(0)}$ was computed to satisfy the condition at $x = 0$, and clearly $\eta^{(1)}$ also satisfies Eq. (3.2a). Inserting $\eta^{(0)} + \eta^{(1)}$ defined by Eqs. (6.5) and (6.7) into condition (3.2b), we obtain

$$k = -[c_1\eta^{(0)}(1) + c_2\eta^{(0)\prime}(1)]/(c_1 + 2c_2), \tag{6.8}$$

where the numerator is known from previous calculations. Inserting Eq. (6.7) into (6.4) we get for the correction for the eigenvalue

$$\sigma^{(1)} = kD, \tag{6.9}$$

where

$$D = (\eta^{(0)}, \eta^{(0)})^{-1}\,[(L_1x^2, \eta^{(0)}) - \sigma^{(0)}(x^2, \eta^{(0)})]. \tag{6.10}$$

Let us define the iteration function

$$\lambda_{(j+1)} = \lambda_{(j)} + k_{(j)}D, \qquad j = 1, 2,..., \tag{6.11}$$

where j counts the iterations. For economy sake, D is not recomputed for every iteration. The initial approximation, as was mentioned before, is

$$\lambda_{(1)} = \lambda(1). \tag{6.12}$$

and the $k_{(j)}$'s are computed by an equation similar to Eq. (6.8), where the values of the eigenfunction and its derivative at $x = 1$ are computed by integrating Eqs. (3.17, 3.18, 3.21, 3.22) with λ replaced by $\lambda_{(j)}$ and $t = 1$. If the initial approximation (6.12) is sufficiently close to its corresponding eigenvalue, i.e., if $\lambda^{(i)}(1)$ is in the domain of attraction of $\lambda_1^{(i)}$, then the iterations will converge.

In order to demonstrate the scheme, we return to the example of the Bessel equation, Eqs. (4.1, 4.2). Since in this case $c_2 = 0$, it follows from Eq. (6.8) that

$$k_{(j)} = -y_{(j)}(1), \tag{6.13}$$

where $y_{(j)}$ is the j-th iterate of the eigenfunction. Also, inserting Eq. (4.1) into (6.10), we obtain

$$D = -\int_0^1 (4x + \lambda_{(1)}x^3)\, y_{(1)}(x)\, dx \Big/ \int_0^1 x y_{(1)}^2\, dx. \tag{6.14}$$

A program was written to perform the iterations defined by Eq. (6.11) in double precision arithmetic, and the results for the first four eigenvalues are summarized in Table I. The error is measured by the deviation of $y_{(j)}^{(i)}(1)$ from zero, and we see from the (rounded) results that the convergence is approximately quadratic.

TABLE I

j	$\lambda_{(j)}^{(1)}$	$\log_{10} y_{(j)}^{(1)}(1)$	$\lambda_{(j)}^{(2)}$	$\log_{10} y_{(j)}^{(2)}(1)$
1	5.7830667	−5	30.467446	−3
2	5.783187560644944	−7	30.49007822449753	−3
3	5.783185962947008	−14	30.47126815070438	−7
4	5.783185962946785	−18	30.47126234365985	−13
5	5.783185962946785	−19	30.47126234366208	−18

j	$\lambda_{(j)}^{(3)}$	$\log_{10} y_{(j)}^{(3)}(1)$	$\lambda_{(j)}^{(4)}$	$\log_{10} y_{(j)}^{(4)}(1)$
1	74.769913	−3	138.52465	−2
2	74.88038481770986	−4	137.8671634518661	−2
3	74.88700694357212	−9	139.0444959928239	−5
4	74.88700679069840	−13	139.0402854828901	−8
5	74.88700679069517	−18	139.0402844267089	−12

VII. Discussion

In the present paper we showed how one can solve the eigenvalue problem (2.1–2.3), by first imbedding it in the family (2.4–2.6), and then reformulating it as a seemingly very complicated (but computationally rather simple) initial-value problem. For the self-adjoint case, Eqs. (2.16–2.17) represent a system of first-order, nonlinear, uncoupled ordinary differential equations with given initial values. It was demonstrated how this problem can be solved numerically on a digital computer. The numerical program consists of nested loops, and we take advantage of the fact that the t-integration in the outer loop is performed discretely. We are now trying to solve this problem on our analog computer by integrating Eqs. (3.17–3.24) by a fast integrator and Eqs. (3.26, 3.9) by a slow one.

In many classical methods [1, 2], instead of finding the eigenvalues of differential equations one seeks the eigenvalues of a matrix which approximate the original problem. These methods become more time-consuming and less accurate for high eigenvalues (i.e., large i in Eq. (2.16)). In "shooting" methods [2], on the other hand, one guesses an eigenvalue and then integrates an initial-value problem satisfying one set of boundary conditions [e.g., Eqs. (3.2a)]. The eigenvalues are

then adjusted in order to satisfy the boundary conditions on the other side (i.e., Eq. (2.2b)). A more sophisticated "shooting" variant was developed by Bailey [31] and Godart [32] who used the Prüfer substitution which transforms the Sturm–Liouville problem into a Ricatti equation. This approach was extended and generalized by Scott *et al.* [18], whose method is particularly suitable for evaluating characteristic lengths. After the completion of the present work, Professor Kalaba let me know that he had derived [33] an equation similar to Eq. (2.16) in order to study the changes of the eigenvalues of a matrix due to changes in its elements, (see also [34]). One should note, however, that eigenvalues of a matrix, unlike those of differential equations treated by us, cannot be determined independently, which is a severe drawback.

There are two possible drawbacks to the continuation method. The first is that the solution of some problems may be rather slow. The reason is clear: in effect one has to solve accurately many itermediate problems for $0 < t < 1$, whose solution is usually not of interest, in order to reach the solution of the original problem at $t = 1$. Therefore, it is usually economical to combine this method with efficient iterative schemes, as was done in this work and in [3, 4]. In fact, one does not have to wait until $t = 1$ in order to iterate, but can do so also at intermediate t's [35]. The second difficulty is the possibility of exponential growth of unwanted solutions ("ill-conditioned problems"). This can sometimes be overcome by prescribing greater accuracy in the computations, or more economically, by using a suitable variant, for example, parallel shooting [2]. On the other hand, the main advantages of the present method are that it is suitable for computers, it is non-iterative, and that the eigenvalues are determined independently–a useful property for the next generation parallel computers.

Acknowledgment

The author would like to thank J. McKenna for many helpful discussions, P. Hohenberg and M. Barmatz who provided the motivation for this study, and Miss J. B. Seery who expertly wrote the computer programs. Thanks also go to the referees for their constructive comments.

References

1. L. Collatz, "The Numerical Treatment of Differential Equations," pp. 227–251, Springer-Verlag, Berlin/New York, 1960.
2. H. B. Keller, "Numerical Methods for Two-Point Boundary-Value Problems," especially Chap. 5, Blaisdell, Waltham, MA, 1968.
3. E. Wasserstrom, "Numerical Solutions by the Continuation Method," TAE Report No. 123, Technion, Haifa, Israel, 1971; submitted for publication in *SIAM Rev.*
4. E. Wasserstrom, Root finding of polynomials as an initial value problem, *J. Computational Phys.* **8** (1971), 304–308.

5. E. WASSERSTROM, Solving boundary-value problems by imbedding, *J. Assoc. Comput. Mach.*, to appear.
6. F. A. FICKEN, The continuation method for functional equations, *Comm. Pure Appl. Math.* **4** (1951), 435–456.
7. G. H. MEYER, On solving nonlinear equations with a one-parameter operator imbedding, *SIAM J. Numer. Anal.* **5** (1968), 739–752.
8. P. LAASONEN, An imbedding method of iteration with global convergence, *Computing*, **5** (1970), 253–258.
9. D. F. DAVIDENKO, On a new method of numerical solution of systems of nonlinear equations (in Russian), *Dokl. Akad. Nauk SSSR* **88** (1953), 601–602.
10. D. F. DAVIDENKO, An application of the method of variation of parameters to the construction of iterative formulas of increased accuracy for numerical solutions of nonlinear equations, *Dokl. Akad. Nauk SSSR* **162** (1965), 702–706.
11. M. N. YAKOVLEV, The solution of systems of nonlinear equations by a method of differentiation with respect to a parameter, *USSR Compt. Math. Math. Phys.* **4** (1964), 198–203.
12. R. W. KLOPFSTEIN, Application of differential equations in general problem solving, *Comm. ACM* **8** (1965), 575–578.
13. R. BELLMAN, R. KALABA, AND G. M. WING, Invariant imbedding and mathematical physics—I: Particle processes, *J. Math. Phys.* **1** (1960), 280–308.
14. R. BELLMAN, Invariant imbedding and computational methods in radiative transfer, *in* "Proceedings of the Symposia in Applied Mathematics," Vol. 19, American Mathematical Society, Providence, R.I., 1968.
15. J. L. CASTI, H. H. KAGIWADA, AND R. E. KALABA, "The Invariant Imbedding Numerical Method for Fredholm Integral Equations with Displacement Kernels, RM-5919-PR (1969), The RAND Corporation, 1969.
16. R. HUSS AND R. KALABA, Invariant imbedding and the numerical determination of Green's functions, *J. Optimization Theory Appl.* **6** (1970), 415–423.
17. E. M. SHOEMAKER, Invariant imbedding applied to eigenvalue problems in mechanics, *J. Appl. Mech.* **32** (1965), 4750.
18. M. R. SCOTT, L. F. SHAMPINE, AND G. M. WING, Invariant imbedding and the calculation for eigenvalues for Sturm–Liouville Systems, *Computing* **4** (1969), 19–23.
19. S. GOLDSTEIN, "Modern Developments in Fluid Dynamics," Vol. I, p. 135, Oxford University Press, London, 1957.
20. M. S. KLAMKIN, On the transformation of a class of boundary value problems for ordinary differential equations, *SIAM Rev.* **4** (1962), 43–47.
21. T. Y. NA, Transforming boundary conditions to initial conditions for ordinary differential equations, *SIAM Rev.* **9** (1967), 204–210.
22. G. G. BELFORD, An initial value problem approach to the solution of eigenvalue problems, *SIAM J. Numer. Anal.* **6** (1969), 99–103.
23. E. A. CODDINGTON AND N. LEVINSON, "Theory of Ordinary Differential Equations," Chap. 7, McGraw-Hill, New York, 1955.
24. A. I. FORSYTHE, T. H. KEENAN, E. I. ORGANICK, AND W. STENBERG, "Computer Science: A First Course," p. 171, Wiley, New York, 1969.
26. P. C. CRANE AND P. A. FOX, "DESUB" — Integration of a First Order System of Ordinary Differential Equations," Numerical Mathematics Computer Programs, Vol. 2, No. 1, Bell Telephone Laboratories, Murray Hill, N.J., 1969.
27. J. S. DRANOFF, An eigenvalue problem arising in mass and heat transfer studies, *Math. Comp.* **15** (1961), 403–409.
28. Reference [23, Chap. 12].

29. L. COLLATZ, "Functional Analysis and Numerical Mathematics," Chap. 2, Academic, New York, 1966.
30. T. KATO, "Perturbation Theory for Linear Operators," see Introduction, Spring-Verlag, Berlin/New York, 1966.
31. P. B. BAILEY, Sturm–Liouville via a phase function, *J. SIAM Appl. Math.* **14** (1966), 242–249.
32. M. GODART, An iterative method for the solution of eigenvalue problems, *Math. Comp.* **20** (1966), 399–406.
33. R. KALABA, W. SCHMAEDEKE, AND B. VEREEKE, "Variational Equations for Certain Homogeneous and Inhomogeneous Linear Systems," Memorandum RM-5690-PR (1968), RAND Corp. 1968.
34. R. COURANT AND D. HILBERT. Method of Mathematical Physics," Vol. I., pp. 343–350, Interscience, New York, 1953.
35. E. WASSERSTROM, Numerical solution of initial-value problems whose solution is known implicitly, unpublished, 1971.