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# ON THE MULTIPLICITY OF SOLUTIONS OF A DIFFERENTIAL EQUATION ARISING IN CHEMICAL REACTOR THEORY

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SOLUTIONS OF A DIFFERENTIAL EQUATION

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ABSTRACT

Consider the boundary value problem $y'' + \frac{1}{x} y' + \beta \exp \{- \frac{1}{|y|}\} = 0$ , $y'(0) = 0$ , $y(1) = \tau$ where $\beta \geq 0$ , $\tau \geq 0$ . We are concerned with a mathematically rigorous num erical study of the number of solutions in any bounded portion of the positive quadrant $(\tau \geq 0 , \beta \geq 0)$ of the $\tau , \beta$ plane. These correct computational results may then be matched with asymptotic $(\beta \to \infty , \tau \geq 0)$ results developed earlier.

These numerical results are based on the development of a-posteriori error estimates for the numerical solution of an associated initial value problem and a-priori bounds on

$$\phi_k(x,y_0) = \frac{\partial^k}{\partial y_0} y(x,y_0) .$$

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## 1. Introduction.

In the present paper, we shall be concerned with the multiplicity of the solutions of the following nonlinear boundary-value problem:

$$(1.1)\quad \begin{cases} y'' + \frac{1}{x} y' + \beta \exp\left\{-\frac{1}{|y|}\right\} = 0 , \quad 0 \leqslant x \leqslant 1 \\ y'(0) = 0 , \quad y(1) = \tau \end{cases}$$

where $\tau, \beta \geqslant 0$ are nonnegative parameters.

The problem arises in the study of chemically reacting systems with cylindrical symmetry; y is then essentially the temperature, and $\beta$ is a dimensionless combination of other physical parameters (see Cotter [ 3 ], Gavalas [ 6 ], and Frank-Kamenetskii [ 5 ]).

Some time ago, two of us (M. Stein and P. Stein) undertook extensive computations to study this problem. The calculations (reported in Parter [ 8 ]) confirmed in all essential details the qualitative picture conjectured by Cotter. S. V. Parter [ 8 ] then attacked the problem analytically and succeeded in establishing several important theorems. Parter's work tended to confirm the correctness of Stein and Stein's numerical study, but there remained certain gaps in the picture. Furthermore, the computational results could not be said to have been rigorously justified.

The calculations of Stein and Stein were based on solving the initial value problem implied by (1.1). Unfortunately, the available literature appears to limit the treatment of convergence and error estimates for initial value problems to those cases where a uniform Lipschitz condition exists. Clearly, the Bessel operator appearing in (1.1) admits of no such condition because of the apparent singularity at $x = 0$.

Despite these technical difficulties it was thought worthwhile to attempt a rigorously correct mathematical study of the problem. Our hope - justified, as it turned out - that this could be done was based on the striking agreement of the analytical and computational results for large values of $\beta$. More precisely, the curves in the $\beta, \tau$ plane which separate regions of uniqueness and nonuniqueness (see Fig. 1) are well approximated in an asymptotic sense by Parter's formulas. It remains to remove the discrepancies between the computational and analytic results in a finite portion of the parameter space. To this end, a theory of a posteriori error estimates is developed and applied to the present problem in the range

$$0 \leqslant \beta \leqslant 31.0525 \quad .$$

Rigorously correct error estimates are obtained which complement the results of [ 8 ] and, in effect, serve to justify the original calculations. It should be pointed out that the methods developed here can in principle be applied to a wide range of problems; it is hoped that the present example will convince other workers in the field of the power and utility of these methods.

All computations described in this paper were carried out on the MANIAC at the Los Alamos Scientific Laboratory. They are based on the earlier work of Stein and Stein in the sense that they use precisely the same difference equations to obtain an approximation $\overline{Y}_1(\xi,y_0)$ to the solutions of (1.1).

The computational scheme is described in Section 3. Sections 4 and 5 are devoted to deriving the necessary estimates for the a posteriori error bounds. In Section 6 we show how these estimates and the computational results can be used to establish the conclusions given in Section 3. The concluding Section 7 contains general remarks.

2. The computation.

Let

$$(2.1)\qquad f(y) = \frac{e^2}{4}\exp\left\{-\frac{1}{|y|}\right\} .$$

Let

$$(2.2a)\qquad \bar{\beta} = 4\,\beta/e^2 \quad , \quad \xi = \sqrt{\bar{\beta}}\; x \quad ,$$

$$(2.2b)\qquad Y(\xi) = y(x) \quad .$$

Then problem (1.1) becomes

$$(2.3)\qquad \begin{cases} \dfrac{d^2}{d\xi^2}Y + \dfrac{1}{\xi}\dfrac{dY}{d\xi} + f(Y) = 0 \;, & 0 \leqslant \xi \leqslant \sqrt{\bar{\beta}} \\[2ex] \dfrac{dY}{d\xi}(0) = 0 \;, \quad Y\left(\sqrt{\bar{\beta}}\right) = \tau . \end{cases}$$

Obviously, every solution of the boundary-value problem (2.3) is also the solution of some initial value problem of the form

$$(2.4)\qquad \begin{cases} \dfrac{d^2}{d\xi^2}Y + \dfrac{1}{\xi}\dfrac{dY}{d\xi} + f(Y) = 0 \;, & 0 \leqslant \xi \leqslant \sqrt{\bar{\beta}} \\[2ex] \dfrac{dY}{d\xi}(0) = 0 \;, \quad Y(0) = y_0 \end{cases}$$

for some choice of $y_0$. Thus, the plan of the computation is the following:

(i) Solve the initial-value problem (2.4) for all choices of $y_0$, $0 \leqslant y_0 < \infty$ .

(ii) For fixed values of $\xi_0$, study the function $Y(\xi_0, y_0)$ as a function of $y_0$.

(iii) For any given value of $\tau$, the number of solutions, $y_0$, of

$$(2.5)\qquad Y\left(\sqrt{\bar{\beta}}, y_0\right) = \tau$$

is exactly the number of solutions of the boundary-value problem (1.1).

Quite clearly we cannot hope to carry out this program for all $\overline{\beta}$, $0 \leqslant \overline{\beta} < \infty$ and all $y_0$, $0 \leqslant y_0 < \infty$. However, since the analytic results of [8] are quite good for large $\beta$, we may restrict $\beta$ to some finite interval. Based on the results of [8] we choose the range

(2.6a) $\quad 0 \leqslant \beta \leqslant 31.0525$

which corresponds to

(2.6b) $\quad 0 \leqslant \xi \leqslant 4.1 \quad .$

This choice of $\beta$ is based on the desire to extend the region $R'$ of [8] in which there are at least three solutions of the boundary-value problem (1.1).

If we were only concerned with an improvement of the uniqueness results of [8], it would be sufficient to limit ourselves to the interval

(2.7a) $\quad 0 \leqslant \beta \leqslant 16.959546$

which corresponds to

(2.7b) $\quad 0 \leqslant \xi \leqslant 3.03 \quad .$

As we shall see in Section 6, our computational results show that this smaller range of $\beta$ is enough to determine our range of $y_0$. We recall two results of [8].

Lemma 2.1. Let $\overline{\alpha}$ have the property that

(2.8) $$17 \exp\left\{\frac{-1}{\alpha + 0.25}\right\} < 4\alpha\,, \quad \overline{\alpha} < \alpha \quad .$$

Let

(2.9) $\quad 0 \leqslant \beta \leqslant 17\,, \quad 0 \leqslant \tau \leqslant 1/4$

and let $y(x\,;\beta,\tau)$ be a solution of the boundary value problem (1.1). Then

(2.10) $$y(0\,;\beta,\tau) \leqslant \overline{\alpha} + \tau \leqslant \overline{\alpha} + 0.25 \quad .$$

Proof. See [8, lemma 5.4].

Corollary 2.1. Let

(2.11a) $\quad 4.2 \leqslant y_0 \quad .$

Let $Y(\xi,y_0)$ be the solution of the initial-value problem (2.4). Then

(2.11b) $\quad Y(\xi,y_0) \geqslant 1/4 \,, \quad 0 \leqslant \xi \leqslant 3.03 \quad .$

Proof: Computational results show that we may take

$$\bar{\alpha} = 3.2 \quad .$$

Thus, inequality (2.11b) follows from the remark that every solution of the boundary-value problem is the solution of an appropriate initial-value problem and vice-versa.

Lemma 2.2: If

$$\tau \geqslant 1/4$$

there is one and only one solution of the boundary value problem (1.1).

Proof: See [ 8 ; Corollary 5.3.2, Theorem 5.1].

Thus, we restrict the computation to the range

(2.12) $\quad 0 \leqslant y_0 \leqslant 4.2 \quad .$

Of course, for a fixed $y_0$ we cannot obtain $Y(\xi,y_0)$ with complete accuracy. Thus we require precise error estimates for the "approximate solution," $\bar{Y}(\xi,y_0)$. Such estimates are discussed in Section 5. Moreover, we cannot obtain "approximate solutions" for all choices of $y_0$. Hence, we require precise error estimates on intermediate values of $y_0$. Such estimates are also discussed in Section 5.

The computations were carried out with

(2.13) $$\begin{cases} \Delta y_0 = 0.0125 \,, & 0 \leqslant y_0 \leqslant 1 \\ \Delta y_0 = 0.0250 \,, & 1 < y_0 \leqslant 4.2 \quad . \end{cases}$$

In principle we have $\overline{Y}(\xi,y_0)$ for all values of $\xi$. Nevertheless, we only sampled this data at intervals with $\Delta\xi = 0.01$. However, we know that

$$\left| \frac{\partial^2 Y}{\partial \xi^2} \right| \leqslant \frac{\xi}{2} \frac{e^2}{4}$$

and $\frac{\partial Y}{\partial \xi} \leqslant 0$. Thus we can also easily estimate the error in intermediate points as in Theorem 5.1.

Having said all this, we now turn to the actual computions. Despite the lack of a uniform Lipschitz condition we employ a standard fourth order Runge-Kutta method for differential equations of the second order (see Collatz [ 2 , Table II/5, page 69]) with a step size of

$$(2.14) \qquad h = 0.01 \quad .$$

On each interval of length h, say $[kh, (k+1)h]$, we use the values $Y_k$, $Y_k'$, $Y_k''$, $Y_{k+1}$, $Y_{k+1}'$, $Y_{k+1}''$ (note: $Y_j''$ is determined from the differential equation) to interpolate a polynomial $Q(\xi)$ of degree at most five (see Davis [ 4 , page 37]). Patching these polynomials we obtain a function $\overline{Y}(\xi,y_0) \in C^2[0, 4.1]$ which is a polynomial of degree at most five on each interval.

In order to apply the estimates developed in Sections 4 and 5 it is necessary that we have accurate bounds on the residual

$$(2.15) \qquad R(\xi,y_0) = \frac{d^2}{d\xi^2} \overline{Y}(\xi,y_0) + \frac{1}{\xi} \frac{d}{d\xi} \overline{Y}(\xi,y_0) + f\left(\overline{Y}(\xi,y_0)\right) \quad .$$

In order to do this it became necessary to carry out the entire computation in double precision. Nevertheless, a comparison with single precision Runge-Kutta runs showed that the single precision computations of $\overline{Y}(\xi,y_0)$ are sufficiently accurate. Hence, if we had not desired an accurate estimate of

$$\mathrm{Max}\, |R(\xi,y_0)| \quad ,$$

the computation could have been carried out in single precision.

## 3. Results.

First we recall the analytic results of [ 8 ]. Consider the region R″ bounded by the curves

$$C_1:\quad \beta = \frac{\Lambda_0}{2}\left\{(1-2\tau) - \sqrt{1-4\tau}\right\}\exp\left[\frac{2}{1-\sqrt{1-4\tau}}\right], \qquad 0 \leqslant \tau \leqslant 0.20$$

$$C_2:\quad \begin{cases} \beta = \dfrac{\Lambda_0}{2}\left\{(0.6) - \sqrt{0.2}\right\}\exp\left[\dfrac{2}{1-\sqrt{0.2}}\right], & 0.20 \leqslant \tau \leqslant 0.25 \\ \quad \doteq 16.4628344, & 0.20 \leqslant \tau \leqslant 0.25 \end{cases}$$

$$C_3:\quad \tau = 0.25\,, \qquad \frac{\Lambda_0}{4}e^2 \leqslant \beta \leqslant 16.4628344$$

$$C_4:\quad \beta = \frac{\Lambda_0 e^2}{4}\,, \qquad 0 \leqslant \tau \leqslant 0.25$$

where

$$\text{(3.1)}\qquad \Lambda_0 \doteq 5.78305\,,$$

$$\text{(3.2)}\qquad \frac{\Lambda_0 e^2}{4} \doteq 10.68282\,.$$

Lemma 3.1. If $(\tau,\beta) \notin R''$, and $\tau \geqslant 0$, then there is a unique solution of the boundary-value problem (1.1).

Proof: See [ 8 ], Section 6.

Consider the region R′ bounded by the two curves

$$\Gamma_1:\quad \beta = \frac{4}{2}\left\{[1-2\tau] - \sqrt{1-4\tau}\right\}\exp\left[\frac{2}{1-\sqrt{1-4\tau}}\right], \qquad 0 \leqslant \tau \leqslant \tau_0^*$$

$$\Gamma_2:\quad \beta = 2e\left\{(1-2\tau) + \sqrt{1-4\tau}\right\}\exp\left[\frac{2}{1+\sqrt{1-4\tau}}\right], \qquad 0 \leqslant \tau \leqslant \tau_0^*$$

where $\tau_0^*$ is the point where $\Gamma_1$ and $\Gamma_2$ intersect. Computational results show that

$$\tau_0^* \doteq 0.15904$$

$$\Gamma_1(\tau_0^*) = \Gamma_2(\tau_0^*) \doteq 24.325$$

$$\Gamma_2(0) = 4e^2 \doteq 29.556 \quad .$$

Lemma 3.2. If $\tau \geqslant 0$ and $\tau \in \bar{R}'$, the closure of $R'$, then there are at least three solutions of the boundary-value problem (1.1).

Proof: See [ 8 ], Theorem 4.3.

Turning now to the results obtained from these computations we obtain the following theorems. Consider the region $R_-$ bounded by

($\alpha$) the piecewise-linear function $Q_+(\tau)$ given in Table (3.3+)

($\beta$) $\beta = \frac{S_-(\tau)}{2} \left\{(1 - 2\tau) - \sqrt{1-4\tau}\right\} \exp\left[\frac{2}{1 - \sqrt{1-4\tau}}\right]$

where $S_-(\tau)$ is the slowly varying function given in Table (3.4)

($\gamma$) $\beta = 31.0525$.

Theorem 3.1. If $\tau \geqslant 0$ and $(\tau,\beta) \in R_-$, then there exist at least three solutions of the boundary value problem (1.1).

Proof: See Section 6.

Consider the region $R_+$ bounded by

($\alpha$) The piecewise-linear function $Q_-(\tau)$ given in Table (3.3-)

($\beta$) $\beta = \frac{S_+(\tau)}{2} \left\{(1 - 2\tau) - \sqrt{1-4\tau}\right\} \exp\left[\frac{2}{1 - \sqrt{1-4\tau}}\right]$

where $S_+(\tau)$ is the slowly varying function given in Table (3.4).

Theorem 3.2. If $\tau \geqslant 0$, $\beta \leqslant 16.625376$, and $(\tau,\beta) \notin R_+$, then there is one and only one solution of the boundary value problem (1.1).

Proof: See Section 6.

Remark: The results stated above are illustrated in Fig. 1. The region marked "overlap region" is the region in which both the computational results and the analytic results assert the existence of at least three solutions of the boundary-value problem (1.1). Similarly, the results of Theorem 3.2 improve the uniqueness results of [ 8 ] by removing the "kink" in the corner, $0.20 \leqslant \tau \leqslant 0.25$, and raising the lower boundary of $R''$.

Table (3.3-) shows $Q_-(\tau)$. This is a piecewise-linear function which may be taken linear between the indicated values of the argument $\tau$. These arguments are <u>not</u> equally spaced because the computations are actually carried out for equally spaced arguments in $\beta$. The arguments in $\tau$ are then given by $\tau(\beta) - \sigma$, where $\sigma$ is a computed error bound. Moreover, we have not listed all the data obtained from these calculations. We have emphasized the regions $\tau \approx 0.24$ and $\tau \approx 0$ because of their intrinsic interest. Similarly, Table (3.3+) shows $Q_+(\tau)$, which is computed in the same way. Table (3.3M) then shows both functions evaluated at the same representative points.

| $\tau$ | $Q_-(\tau)$ |
|---|---|
| - 0.0137 | 17.07167 |
| - 0.0022 | 16.84779 |
| 0.0034 | 16.73640 |
| 0.0090 | 16.62530 |
| 0.0201 | 16.40444 |
| 0.0311 | 16.18499 |
| 0.0418 | 15.96701 |
| 0.0523 | 15.75050 |
| 0.0627 | 15.53550 |
| 0.1021 | 14.69020 |
| 0.1251 | 14.17400 |
| 0.1550 | 13.46655 |
| 0.1785 | 12.87470 |
| 0.1965 | 12.39163 |
| 0.2079 | 12.10623 |
| 0.2232 | 11.63795 |
| 0.2260 | 11.54540 |
| 0.2287 | 11.45322 |
| 0.2314 | 11.36141 |
| 0.2339 | 11.26997 |
| 0.2364 | 11.17890 |
| 0.2387 | 11.08820 |
| 0.2407 | 10.99787 |

Table 3.3-

| $\tau$ | $Q_+(\tau)$ |
|---|---|
| - 0.0101 | 17.07167 |
| 0.0014 | 16.84779 |
| 0.0070 | 16.73640 |
| 0.0126 | 16.62530 |
| 0.0238 | 16.40444 |
| 0.0347 | 16.18499 |
| 0.0454 | 15.96701 |
| 0.0559 | 15.75050 |
| 0.0663 | 15.53550 |
| 0.1057 | 14.69020 |
| 0.1287 | 14.17400 |
| 0.1586 | 13.46655 |
| 0.1821 | 12.87470 |
| 0.2001 | 12.39163 |
| 0.2087 | 12.10623 |
| 0.2240 | 11.63795 |
| 0.2268 | 11.54540 |
| 0.2291 | 11.45322 |
| 0.2322 | 11.36141 |
| 0.2347 | 11.26997 |
| 0.2372 | 11.17890 |
| 0.2395 | 11.08820 |
| 0.2415 | 10.99787 |

Table 3.3+

| $\tau$ | $Q_-(\tau)$ | $Q_+(\tau)$ |
|---|---|---|
| 0.000 | 16.804029 | 16.875045 |
| 0.005 | 16.704657 | 16.776182 |
| 0.010 | 16.605403 | 16.676882 |
| 0.015 | 16.505916 | 16.577973 |
| 0.020 | 16.406430 | 16.479375 |
| 0.030 | 16.206935 | 16.279615 |
| 0.040 | 16.003680 | 16.077019 |
| 0.050 | 15.797926 | 15.872158 |
| 0.100 | 14.735254 | 14.812490 |
| 0.150 | 13.584811 | 13.669995 |
| 0.160 | 13.340585 | 13.431244 |
| 0.180 | 12.834442 | 12.927584 |
| 0.190 | 12.566053 | 12.662673 |
| 0.200 | 12.303977 | 12.394284 |
| 0.210 | 12.041937 | 12.066418 |
| 0.220 | 11.735924 | 11.760405 |
| 0.230 | 11.409000 | 11.426548 |
| 0.235 | 11.229916 | 11.259068 |
| 0.240 | 11.029505 | 11.065625 |

Table 3.3M

Table (3.4) shows $S_-(\tau)$ and $S_+(\tau)$. These are slowly varying functions which may be taken as piecewise linear between the indicated values of $\tau$. Once more, we have chosen to list only sample values with the most frequent values of $\tau$ in the region of interest, $\tau \approx 0.24$.

| $\tau$ | $S_-(\tau)$ | $S_+(\tau)$ |
|---|---|---|
| 0.17732 | 5.51433 | 5.59805 |
| 0.18403 | 5.53041 | 5.60575 |
| 0.19202 | 5.54498 | 5.61139 |
| 0.21475 | 5.59254 | 5.63862 |
| 0.21864 | 5.60080 | 5.64393 |
| 0.22032 | 5.60548 | 5.64739 |
| 0.22117 | 5.60712 | 5.64841 |
| 0.22204 | 5.60895 | 5-64961 |
| 0.22295 | 5.61193 | 5.65195 |
| 0.22386 | 5.61399 | 5.65337 |
| 0.22479 | 5.61612 | 5.65484 |
| 0.22576 | 5.61921 | 5.65726 |
| 0.22673 | 5.62130 | 5.65868 |
| 0.22878 | 5.62746 | 5.66344 |
| 0.23094 | 5.63404 | 5.66855 |
| 0.23323 | 5.64128 | 5.67425 |
| 0.23444 | 5.64557 | 5.67774 |
| 0.23570 | 5.65040 | 5.68173 |
| 0.23701 | 5.65561 | 5.68605 |
| 0.23838 | 5.66138 | 5.69090 |
| 0.23984 | 5.66858 | 5.69711 |
| 0.24141 | 5.67752 | 5.70497 |

Table 3.4

## 4. A basic estimate.

In this Section we develop the basic mathematical estimate required to establish our a posteriori error bounds.

Suppose $E(\xi)$ is a solution of the initial-value problem

$$(4.1) \qquad \begin{cases} E'' + \frac{1}{\xi} E' + F E = R \ , & 0 < \xi \leqslant A \\ E(0) = E'(0) = 0 \ . \end{cases}$$

Then, after two straightforward integrations we see that

$$(4.2a) \qquad E(\xi) = - \int_0^\xi K(\xi,t)\, F(t)\, E(t)\, dt + \int_0^\xi K(\xi,t)\, R(t)\, dt$$

where

$$(4.2b) \qquad K(\xi,t) = \xi \ln \xi/t \ .$$

That is, if

$$Q(\xi) = \int_0^\xi K(\xi,t)\, G(t)\, dt \ , \qquad 0 < \xi \leqslant A$$

then $Q(\xi)$ is a solution of the initial-value problem

$$(4.3) \qquad \begin{cases} Q'' + \frac{1}{\xi} Q' = G \ , & 0 < \xi \leqslant A \\ Q(0) = Q'(0) = 0 \ . \end{cases}$$

Lemma 4.1. Let

$$(4.4) \qquad K_0(\xi) \equiv 1 \ ,$$

and, for all $j \geqslant 1$, define $K_j(\xi)$ by the recursion

$$(4.5a) \qquad K_j(\xi) = \int_0^\xi K(\xi,t)\, K_{j-1}(t)\, dt \ .$$

Then

$$(4.5b) \qquad K_j(\xi) = \left(\frac{\xi}{2}\right)^{2j} \frac{1}{[j!]^2} , \qquad j = 0, 1, \ldots .$$

Proof: We proceed by induction. By assumption (4.4), Equation (4.5b) holds for $j = 0$. Assume (4.5b) holds for $j = 0, 1, \ldots (J - 1)$. Then, according to (4.3) and (4.5a) we have

$$(\xi K_J')' = \xi K_{J-1} = \frac{(\xi)^{2J-1}}{(4)^{(J-1)}} \left[\frac{1}{(J-1)!}\right]^2 .$$

Thus, Equation (4.5b) follows from a direct integration and the boundary conditions of (4.3).

Corollary: Let $K_j(\xi)$ be defined as above. Then

$$(4.6) \qquad \sum_{j=0}^{\infty} K_j(\xi) = I_0(\xi)$$

where $I_0(\xi)$ is the modified Bessel function of zero$^{th}$ order.

Proof: See page 375, formula 9.6.12 of Abramowitz and Stegun [ 7 ].

Theorem 4.1. Suppose

$$(4.7a) \qquad |F(\xi)| \leqslant M , \qquad 0 \leqslant \xi \leqslant A .$$

Then, for $0 \leqslant \xi \leqslant A$, we have

$$(4.7b) \qquad |E(\xi)| \leqslant \frac{\left[I_0(\sqrt{M}\,\xi) - 1\right]}{M} \cdot \sup\{|R(t)| ; \quad 0 \leqslant t \leqslant \xi\} .$$

Proof: For any function $\alpha(t) \in C\,[0, A]$ let

$$(4.8) \qquad \|\alpha\|(\xi) \equiv \sup\{\alpha|(t)| ; \ 0 \leqslant \xi \leqslant A\} .$$

From (3.2a) we obtain

$$|E(t)| \leqslant \{M\|E\|(t) + \|R\|(t)\} \cdot K_1(t)$$

$$|E(t)| \leqslant \{M\|E\|(\xi) + \|R\|(\xi)\} \cdot K_1(t) , \qquad 0 \leqslant t \leqslant \xi .$$

We proceed by induction. Assume

$$(4.9) \qquad |E(t)| \leqslant K_n(t)M^n \|E\|(\xi) + \left[\sum_{j=1}^{n} M^{j-1}K_j(t)\right] \|R\|(\xi) , \quad 0 \leqslant t \leqslant \xi .$$

Then, using (4.2a) we obtain

$$|E(s)| \leqslant M^{n+1} \|E\|(s) \int_0^s K(s,t)\, K_n(t)\, dt$$

$$+ M\|R\|(\xi) \int_0^s K(s,t) \left[\sum_{j=0}^{n} M^{j-1} K_j(t)\right] dt$$

$$+ \|R\|(\xi)\, K_1(t) .$$

Hence inequality (3.9) holds for all n. Letting $n \to \infty$ we obtain

$$|E(t)| \leqslant \frac{1}{M} \left[\sum_{j=1}^{\infty} M^j K_j(t)\right] \|R\|(\xi) , \qquad 0 \leqslant t \leqslant \xi .$$

That is, (4.7b) holds.

Remark: We observe that

$$\frac{\partial}{\partial M} \left[\frac{I_0(\sqrt{M}\,x) - 1}{M}\right] > 0 \quad \text{for} \quad x > 0 .$$

## 5. Estimates: a priori and a posteriori.

We are concerned with the functions $Y(\xi,y_0)$, $\phi_1(\xi,y_0)$, $\phi_2(\xi,y_0)$ which satisfy the initial value problem

$$(5.1)\qquad \begin{cases} Y'' + \frac{1}{\xi} Y' + f\big(Y(\xi,y_0)\big) = 0 , & 0 < \xi \leq A , \\ \phi_1'' + \frac{1}{\xi}\phi_1' + f'\big(Y(\xi,y_0)\big)\phi_1 = 0 , & 0 < \xi \leq A , \\ \phi_2'' + \frac{1}{\xi}\phi_2' + f'\big(Y(\xi,y_0)\big)\phi_2 + f''\big(Y(\xi,y_0)\big)\phi_1^2 = 0 , & 0 < \xi \leq A , \\ Y'(0,y_0) = \phi_1'(0,y_0) = \phi_2'(0,y_0) = 0 , \\ Y(0,y_0) = y_0 , \quad \phi_1(0,y_0) = 1 , \quad \phi_2(0,y_0) = 0 , \end{cases}$$

where

$$(5.2)\qquad 0 \leq f'(y) \leq 1 , \quad f(y) \geq 0 .$$

We first seek a priori estimates for $\phi_1(\xi,y_0)$ and $\phi_2(\xi,y_0)$. We have

$$(5.3)\qquad \phi_1'(\xi,y_0) = -\frac{1}{\xi}\int_0^\xi t\, f'\big(Y(t,y_0)\big)\,\phi_1(t,y_0)\,dt .$$

Since $\phi_1(0,y_0) = 1$ we see that there is a largest interval $(0,\xi_1)$ such that

$$(5.4a)\qquad 0 \leq \phi_1(\xi,y_0) \leq 1 , \qquad 0 \leq \xi \leq \xi_1 ,$$

and

$$(5.4b)\qquad \phi_1'(\xi,y_0) < 0 , \qquad 0 \leq \xi \leq \xi_1 .$$

Indeed, if $\xi_1 < A$, then

$$(5.4c)\qquad \phi_1(\xi_1,y_0) = 0 ,$$

and there is a largest $\xi_2$, with $\xi_1 < \xi_2 \leq A$ such that the inequality (5.4b) holds on the open interval $(0,\xi_2)$.

Suppose $\xi_1 < A$, then using (5.3) we obtain

$$|\phi_1'(\xi_1,y_0)| \leq \frac{1}{2}\xi_1 \max\{ f'(y) ; y(\xi_1) \leq y \leq y_0 \} . \tag{5.5}$$

We wish to estimate $\xi_1$. We apply the oscillation theorem and compare $\phi_1(\xi,y_0)$ with $J_0(\xi)$ which satisfies

$$\begin{cases} J_0'' + \frac{1}{\xi} J_0' + J_0 = 0 , & 0 < \xi \\ J_0'(0) = 0 , \ J_0(0) = 1 . & \end{cases}$$

Let $r_0$ be the first zero of $J_0(\xi)$. Using the comparison theorems (see Ince [ 7 ]) and the tables of Abramowitz and Stegun [ 1 ] we find that

$$\xi_1 \geq r_0 \doteq 2.4048255 .$$

Suppose $r_1$ is the second zero of $J_0(\xi)$ and

$$A < r_1 \doteq 5.520078 .$$

Then the oscillation theorems imply that

$$\phi_1(\xi,y_0) < 0 , \qquad \xi_1 < \xi \leq A .$$

Moreover, on the interval $(\xi_1,\xi_2)$ we have

$$\phi_1'(\xi,y_0) < 0 , \quad \phi_1(\xi,y_0) < 0 .$$

Thus

$$\phi_1''(\xi,y_0) > 0 , \qquad \xi_1 < \xi < \xi_2 .$$

Since $\xi_2$ is the point in the interval $(\xi_1,A)$ at which $\phi_1(\xi,y_0)$ assumes its minimum, the convexity of $\phi_1$ over that interval gives us the estimate

$$\phi_1'(\xi_1,y_0)(\xi_1 - \xi_0) \leq \phi_1(\xi,y_0) , \qquad \xi_1 \leq \xi \leq \xi_2 .$$

In fact,

$$\phi_1'(\xi_1,y_0)(A - \xi_1) \leqslant \phi_1(\xi,y_0) \leqslant 0 , \qquad \xi_1 \leqslant \xi \leqslant \xi_2 .$$

Applying Theorem 4.1 we obtain the following estimates.

Lemma 5.1. Suppose $y(\xi,y_0)$, $\phi_1(\xi,y_0)$, $\phi_2(\xi,y_0)$ solve the initial-value problem (5.1) where (5.2) holds. Suppose

$$(5.6) \qquad 0 \leqslant A < 2\, r_0 = 4.809651$$

and let

$$(5.7a) \qquad B(y_0) = \max\{|f'(y)| ; \ Y(A) \leqslant y \leqslant y_0\} .$$

$$(5.7b) \qquad \sigma(y_0) = \max\{1, \tfrac{1}{2}\, r_0\, B(y_0)\, [A - r_0]\} .$$

Then, using (5.5) and the fact that $\xi_1 > r_0$, we see that $|\phi_1(\xi,y_0)| \leqslant \frac{1}{2}\, \xi_1 (A - \xi_1)$, whence

$$(5.8) \qquad |\phi_1(\xi,y_0)| \leqslant \sigma(y_0) , \qquad 0 \leqslant \xi \leqslant A .$$

Moreover, let

$$(5.9) \qquad S(y_0) = \max\{|f''(y)| ; \ Y(A) \leqslant y \leqslant y_0\} .$$

Then

$$(5.10) \qquad |\phi_2(\xi,y_0)| \leqslant \frac{\left[I_0(\sqrt{B(y_0)}\ A) - 1\right]}{B(y_0)}\, S(y_0)\, \sigma(y_0)^2 .$$

In our case we are interested in the function

$$(5.11) \qquad f(y) = \frac{e^2}{4} \exp\left\{- \frac{1}{|y|}\right\} .$$

Then

$$(5.12) \qquad |f'(y)| \leqslant 1$$

(5.13) $\quad |S(y_0)| \leqslant \max |f''(y)| \doteq 4.71045 \quad .$

Additional particular estimates which we will use in Section 6 are summarized in the following tables of bounds.

(5.14)

| $0 \leqslant A \leqslant 3.00$ , all $y_0$ | |
|---|---|
| FUNCTION | BOUND |
| $B(y_0)$ | 1 |
| $\sigma(y_0)$ | 1 |
| $\lVert \phi_1(\cdot, y_0) \rVert (A)$ | 1 |
| $I_0\left(\sqrt{B(y_0)}\ A\right)$ | 4.89 |
| $\lVert \phi_2(\cdot, y_0) \rVert (A)$ | 19.5 |

(5.15)

| $0 \leqslant A \leqslant 3.2$ , all $y_0$ | |
|---|---|
| FUNCTION | BOUND |
| $B(y_0)$ | 1 |
| $\sigma(y_0)$ | 1 |
| $\lVert \phi_1(\cdot, y_0) \rVert (A)$ | 1 |
| $I_0\left(\sqrt{B(y_0)}\ A\right)$ | 5.75 |
| $\lVert \phi_2(\cdot, y_0) \rVert (A)$ | 22.37 |

(5.16)

| $0 \leq A \leq 4.2,\ \lvert y(A,y_0)\rvert \leq y_0,\ 0 \leq y_0 \leq 0.3$ | |
|---|---|
| FUNCTION | BOUND |
| $B(y_0)$ | 0.7332214 |
| $\sigma(y_0)$ | 1.580772 |
| $\lVert \phi_1(\cdot, y_0)\rVert (A)$ | 1.580772 |
| $I_0\left(\sqrt{B}(y_0)\ A\right)$ | 8.027823 |
| $\lVert \phi_2(\cdot, y_0)\rVert (A)$ | 113.028 |

Having obtained these a priori estimates we are now in a position to obtain a posteriori error estimates.

Theorem 5.1: Suppose $\overline{Y}(\xi,y_0)$, $\overline{Y}(\xi,z_0)$ are approximations to $Y(\xi,y_0)$, $Y(\xi,z_0)$ respectively. Let

$$R(\xi,y_0) = \overline{Y}''(\xi,y_0) + \frac{1}{\xi}\overline{Y}'(\xi,y_0) + f\left(\overline{Y}(\xi,y_0)\right) \quad ,$$

$$R(\xi,z_0) = \overline{Y}''(\xi,z_0) + \frac{1}{\xi}\overline{Y}'(\xi,z_0) + f\left(\overline{Y}(\xi,z_0)\right) \quad ,$$

be the corresponding "residuals." Let

$$0 < y_0 < z_0 \quad ,$$

and let

$$C(A) = C(\xi,z_0) = \frac{I_0\left(\sqrt{B(z_0)}\ A\right) - 1}{B(z_0)} \quad .$$

Then, for $0 \leq \xi \leq A$

$$(5.17)\qquad \begin{cases} \lvert Y(\xi,y_0) - \overline{Y}(\xi,y_0)\rvert \leq C(A)\ \lVert R(\cdot, y_0)\rVert (A) \\ \lvert Y(\xi,z_0) - \overline{Y}(\xi,z_0)\rvert \leq C(A)\ \lVert R(\cdot, z_0)\rVert (A) \quad . \end{cases}$$

Moreover, let z be an intermediate point, i.e.,

$$y_0 < z < z_0 \quad ,$$

and let

$$(5.18) \qquad K = \{\max |\phi_2(t,q)| \; ; \qquad 0 \leq t \leq A \, , \quad y_0 \leq q \leq z_0\} \; .$$

Let

$$(5.19) \qquad E = C(A) \cdot \max\{\|R(\cdot, y_0)\|(A) \; , \quad \|R(\cdot, z_0)\|(A)\} \quad .$$

Let

$$(5.20) \qquad \overline{Y}(\xi,z) = \frac{\overline{Y}(\xi,y_0)(z_0 - z) + \overline{Y}(\xi,z_0)(z - y_0)}{z_0 - y_0} \quad .$$

Then

$$(5.21) \qquad |\overline{Y}(\xi,z) - Y(\xi,z)| \leq E + \frac{K}{8}\,|y_0 - z_0|^2 \quad .$$

Proof: The estimates (5.18) follow immediately, Theorem 4.1. The estimate (5.21) follows from a straightforward computation using a Taylor series expansion of $Y(\xi,y_0)$ and $Y(\xi,z_0)$ about z.

## 6. Analysis of the computational results.

Throughout the entire range of calculation we find that

$$(6.1) \qquad |R(\xi,y_0)| \leqslant 2.5 \times 10^{-6} \quad .$$

Since

$$I_0(4.2) < 13.45 \quad ,$$

we have, using Theorem 5.1, all the computed Runge-Kutta approximations $\overline{Y}(\xi_0,y_0)$ satisfy

$$(6.2) \qquad |\overline{Y}(\xi,y_0) - Y(\xi,y_0)| \leqslant (31.13) \times 10^{-6} , \qquad 0 \leqslant \xi \leqslant 4.1 \quad .$$

Studying the functions $\overline{Y}(\xi,y_0)$, as functions of $y_0$, a very definite pattern emerges (see Fig. 2). For small values of $\xi_0 (\leqslant 2.44)$ this function is a monotone increasing function of $y_0$. For slightly larger values of $\xi_0$ the function $\overline{Y}(\xi_0,y_0)$ develops exactly one relative maximum, $\overline{Y}(\xi_0,y_0)_{max}$, and exactly one relative minimum $\overline{Y}(\xi_0,y_0)_{min}$, and continues on as a monotone increasing function. This shape can be described as a (distorted) sidewise S shape. At $\xi_0 = 3.02$ the function assumes negative values. And, for all larger $\xi_0$, we have

$$(6.3) \qquad \overline{Y}(\xi_0,y_0)_{min} < 0 , \qquad \xi_0 \geqslant 3.02 \quad .$$

Thus, for all values of $\tau$ which satisfy

$$(6.4a) \qquad \overline{Y}(\xi_0,y_0)_{min} > \tau \geqslant 0 \quad ,$$

the boundary value problem (1.1) with

$$(6.4b) \qquad \beta = \frac{e^2}{4} \xi_0^2 \quad ,$$

possesses a unique solution. Similarly, for all values of $\tau$ which satisfy

$$(6.5) \qquad \overline{Y}(\xi_0,y_0)_{max} < \tau \quad ,$$

the boundary value problem (1.1), with $\beta$ given by (6.4b), possesses a unique solution. Finally, if $\tau$ satisfies

$$(6.6) \qquad \overline{Y}(\xi_0,y_0)_{\min} < \tau < \overline{Y}(\xi_0,y_0) \quad ,$$

the boundary value problem (1.1), with $\beta$ given by (6.4b), possesses at least three solutions.

Since we are only interested in $\tau \geqslant 0$, for all $\xi_0 \geqslant 3.02$ we obtain a $\tau$ interval in which there are at least three solutions. Thus, as we remarked earlier (Section 2), it is not necessary to consider a larger range of $y_0$ to extend the region in which there exist at least three solutions.

Of course, the remarks above are not strictly true. For example, in (6.4a) we must replace $\overline{Y}(\xi_0,y_0)_{\min}$ by $\left[\overline{Y}(\xi_0,y_0)_{\min} - \sigma\right]$ where $\sigma$ is some accurate bound on

$$(6.7) \qquad |\overline{Y}(\xi_0,y_0)_{\min} - Y(\xi_0,y_0)_{\min}| \quad .$$

Similar modification must be made in the other formulas given above. Moreover, if we could be assured that $\overline{Y}(\xi_0,y_0)$ really has only one maximum and only one minimum we could claim that there are exactly three solutions when (6.6) holds. Since we only obtain bounds, we cannot make such a claim. However in Section 7 we shall make some remarks about the possible extension of these results.

The above remarks indicate that we must obtain precise error bounds on

$$|Y(\xi_0,y_0) - \overline{Y}(\xi_0,y_0)| \quad .$$

Since the analytic results of [8] give good results (one boundary of the uniqueness domain) for $\tau \leqslant 0.20$ which corresponds to $\beta = 16.4628344$, we are interested in $Y(\xi_0,y_0)_{\max}$ for

$$0 \leqslant \xi_0 \leqslant 3.0 \quad .$$

Looking at our results, we see that the critical value of $y_0$ at which $\overline{Y}(\xi,y_0)$ assumes its maximum always satisfies

$$(y_0)_{\max} < 1 \quad .$$

Moreover, the value of $\overline{Y}(\xi,1)$ is sufficiently different (based on (6.2)) from $Y(\xi,y_0)_{max}$ that we may use Theorem 5.1 and estimate (5.21) with

(6.8a) $\quad \Delta y_0 = 0.0125 \quad .$

Thus using Table (5.14) we have

(6.8b) $\quad |\overline{Y}(\xi,y_0)_{max} - Y(\xi,y_0)_{max}| \leqslant 4 \times 10^{-4}, \qquad 0 \leqslant \xi \leqslant 3.0 \quad .$

Then, for each selected value of $\beta$ we solve for $S_-(\tau)$ and $S_+(\tau)$ from the formulas

(6.9a) $$2\beta = S_\pm(\tau) \left\{[1 - 2(\tau \pm \sigma)] - \sqrt{1 - 4(\tau \pm \sigma)}\right\} \exp\left\{ \frac{2}{1 - \sqrt{1 - 4(\tau \pm \sigma)}} \right\}$$

where

(6.9b) $\quad \sigma = 4 \times 10^{-4} \quad .$

Monotonicity properties guarantee that

(6.9c) $\quad S_-(\tau) \leqslant S(\tau) \leqslant S_+(\tau), \qquad 0 \leqslant \tau \leqslant 0.20 \quad .$

Thus we have justified the statemants of Section 3. For larger values of $\beta$ (which correspond to larger values of $\xi_0$) we proceed in the same way, using the estimates of Tables (5.15) and (5.16). It is important to note that the value $(y_0)_{max}$ at which $\overline{Y}(\xi_0,y_0)_{max}$ occurs satisfies

$$(y_0)_{max} \leqslant 0.3 \text{ , } \quad \xi_0 \geqslant 3.0 \quad .$$

Finally we turn to the behavior of $\overline{Y}(\xi_0,y_0)_{min}$ for $0 \leqslant \xi_0 \leqslant 3.02$. Using the Table (5.15), Theorem 5.1 and the data, we find that

$$|\overline{Y}(\xi,y_0)_{min} - Y(\xi,y_0)_{min}| \leqslant \begin{cases} 4 \times 10^{-4} \quad , & \xi \leqslant 2.58 \\ 1.8 \times 10^{-3} \quad , & 2.58 < \xi \quad . \end{cases}$$

Using this estimate we construct $Q_{\pm}(\tau)$ as a piecewise linear function. For example, let $\beta_1, \beta_2$ be two consecutive values of $\beta$ at which we have "sampled" our data. Then

$$Q_{\pm}\left[Y\left(\sqrt{\bar{\beta}_k}, y_0\right)_{min} \pm 1.6 \times 10^{-5}\right] = \frac{e^2}{4}\,\bar{\beta}_k = \beta_k\,, \qquad k = 1, 2 \quad . \tag{6.10}$$

Linear interpolation is then used to obtain $Q_{\pm}(\tau)$ at common values of $\tau$.

## 7. Check calculations and remarks.

While the basic computations of this report were carried out on the MANIAC as described in Section 2, we undertook some additional check calculations.

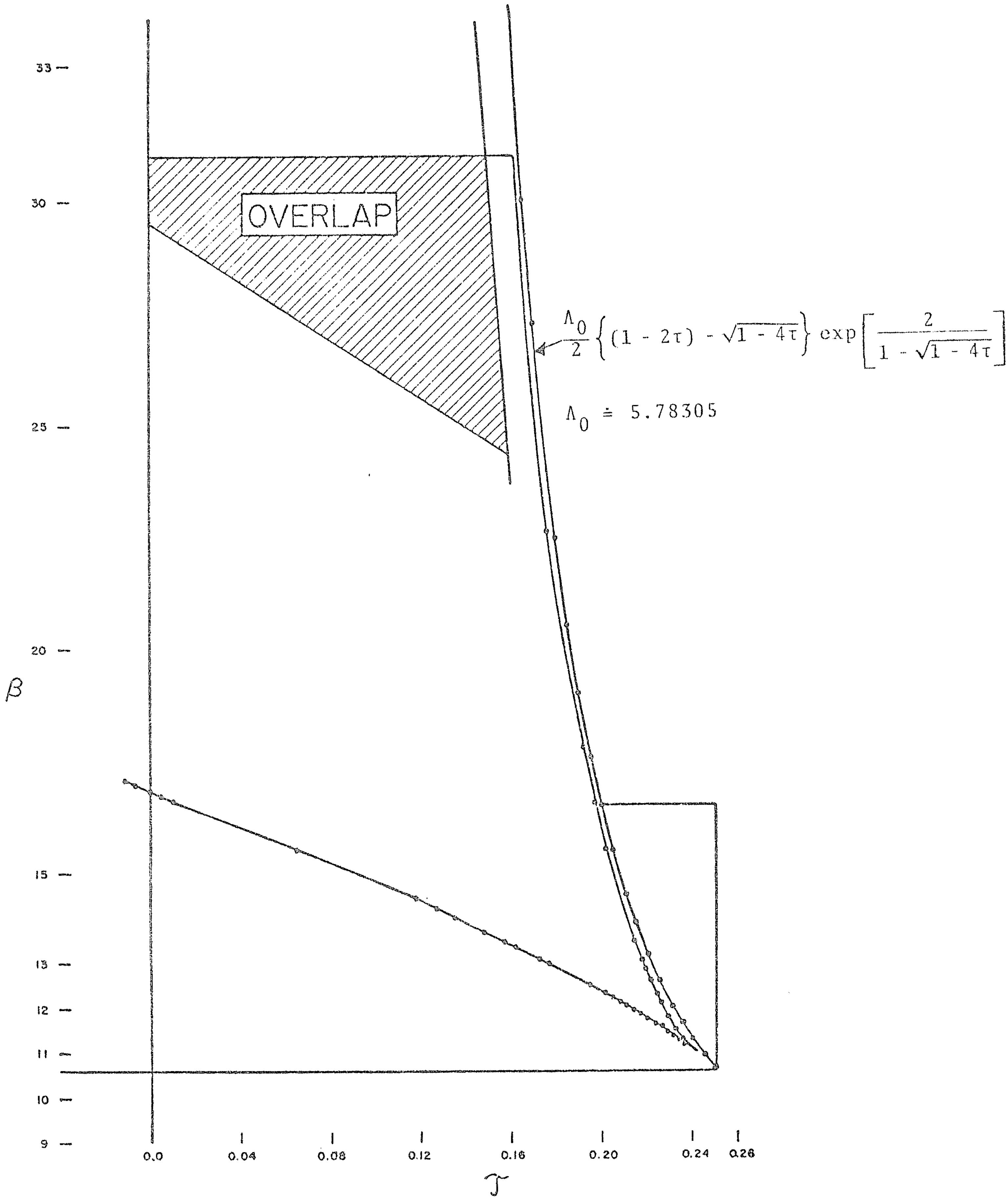
Instead of the Runge-Kutta calculations described in Section 2, consider the following collocation method. On each interval of length h, say $[kh, (k+1)h]$ we determine a quintic polynomial $Q(\xi)$ which satisfies the equation at the four points (Lobatto points)

$$\begin{aligned} \xi_k &= kh , \\ \bar{\xi} &= kh + \frac{h}{10}(5-\sqrt{5}) , \\ \bar{\eta} &= kh + \frac{h}{10}(5+\sqrt{5}) , \\ \xi_{k+1} &= (k+1)h . \end{aligned}$$

As in Section 2, patching this quintic together gives an approximation $\bar{Y}(\xi,y_0)$. This procedure was used on the CDC 7600 for $y_0 = 1, 2, 3, 4$. The results agreed with the Runge-Kutta computations to 6 significant figures and the residuals were noticably smaller. The above "check" calculations were programmed by John Cerutti. We take this opportunity to thank him.

As we commented in Section 6, the computational results seem to imply that our conclusion should be "exactly three solutions" rather than "at least three solutions." If one were willing to undertake the additional calculations, one could use the methods developed in this report to establish such statements. It is necessary to compute $\phi_1(\xi,y_0)$ very accurately. This can be done. However, we have contented ourselves with these more modest results simply because we thought it more important to make the point - the potential of computing for precise results - rather than lose the reader in a maze of technical details. We fear we may have done that even with these limited results.

Finally, we remark that our error bounds clearly overestimate the actual errors. A more careful development of the error estimate of Section 4 would give the error as an integral of a positive kernal and R(t). The estimates of Section 4 replace R(t) by max $|R(t)|$. However, the actual residual of our computations are highly oscillatory functions.



OVERLAP
$\frac{\Lambda_0}{2}\left\{(1-2\tau)-\sqrt{1-4\tau}\right\}\exp\left[\frac{2}{1-\sqrt{1-4\tau}}\right]$
$\Lambda_0 \doteq 5.78305$
33
30
25
20
$\beta$
15
13
12
11
10
9
0.0
0.04
0.08
0.12
0.16
0.20
0.24
0.26
$\tau$


Figure 1.

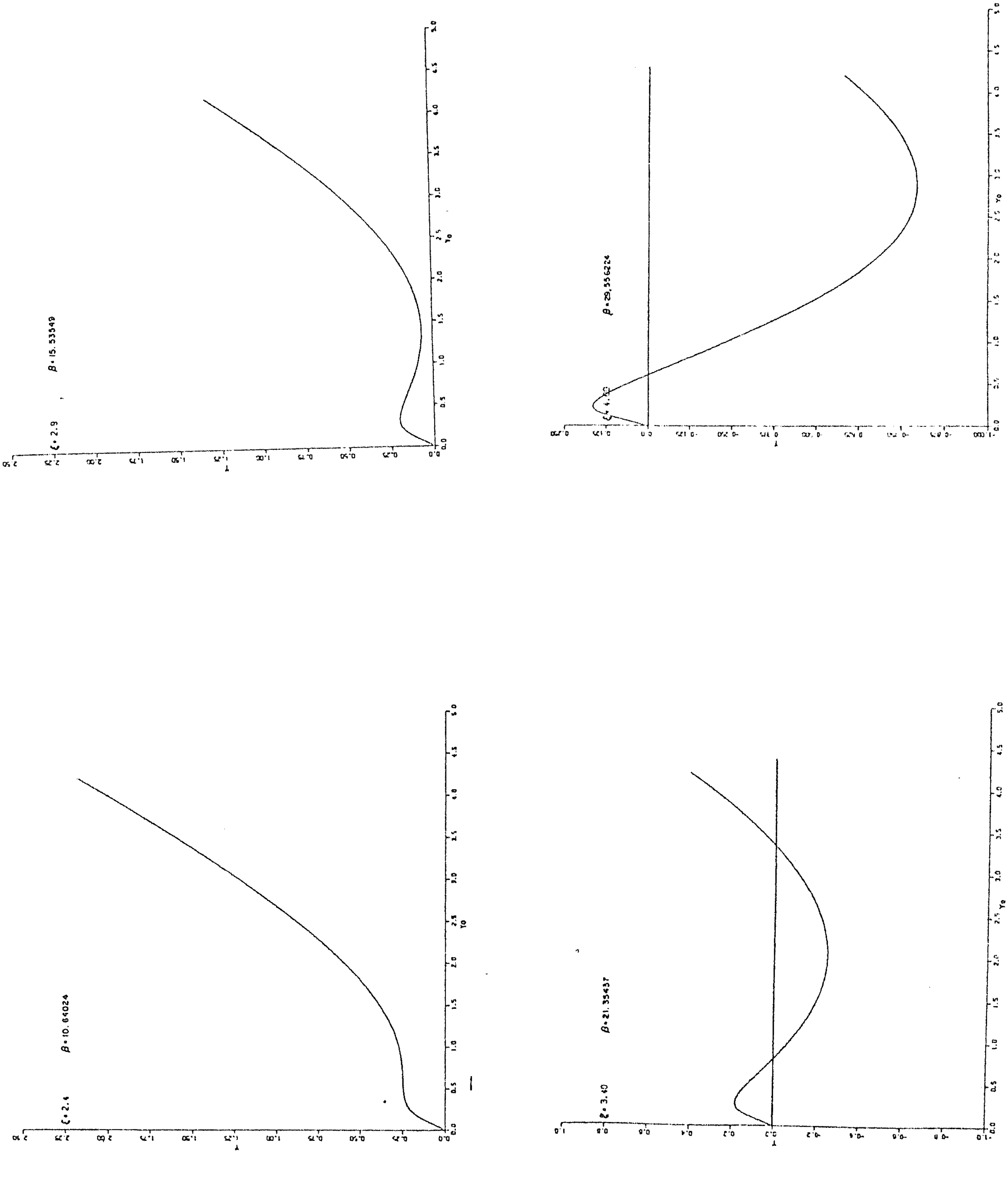



Figure 2.

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13. ABSTRACT

Consider the boundary value problem $y'' + \frac{1}{x} y' + \beta \exp\{-\frac{1}{|y|}\} = 0$, $y'(0) = 0$, $y(1) = \tau$ where $\beta \geq 0$, $\tau \geq 0$. We are concerned with a mathematically rigorous numerical study of the number of solutions in any bounded portion of the positive quadrant $(\tau \geq 0, \beta \geq 0)$ of the $\tau, \beta$ plane. These correct computational results may then be matched with asymptotic $(\beta \to \infty, \tau \geq 0)$ results developed earlier.

These numerical results are based on the development of a-posteriori error estimates for the numerical solution of an associated initial value problem and a-priori bounds on

$$\phi_k(x,y_0) = \frac{\partial^k}{\partial y_0} y(x,y_0) .$$

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| A-posterori Error Estimates | | | | | | |
| Multiplicity of Solutions | | | | | | |