*Math. Proc. Camb. Phil. Soc.* (1997), **121**, 495
*Printed in Great Britain*



# Approximate diagonalization in differential systems and an effective algorithm for the computation of the spectral matrix

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(*Received* 17 *May* 1995; *revised* 22 *January* 1996)

## 1. *Introduction*

In a recent paper [**3**], an extended Liouville–Green formula

$$y(x) = \gamma_M(x)\{1+\epsilon_M(x)\}\exp\left(\pm\int_X^x Q_M(t)\,dt\right) \tag{1·1}$$

was developed for solutions of the second-order differential equation

$$y''(x)-Q(x)\,y(x)=0 \quad (0\leqslant x<\infty). \tag{1·2}$$

Here $\gamma_M(x)\sim Q^{-\frac{1}{4}}(x)$, $Q_M(x)\sim Q^{\frac{1}{2}}(x)$ and $\epsilon_M(x)\to 0$ as $x\to\infty$, while $M\,(\geqslant 2)$ is an integer and $\gamma_M$ and $Q_M$ can be defined in terms of $Q$ and its derivatives up to order $M-1$. The general form of (1·1) had been obtained previously by Cassell [**5**], [**6**], [**7**] and Eastham [**10**], [**11**, section 2·4]. In particular, the proof of (1·1) in [**10**] and [**11**] depended on the formulation of (1·2) as a first-order system and then on a process of $M$ repeated diagonalization of the coefficient matrices in a sequence of related differential systems.

The main contribution of [**3**] to (1·1) was to show that, for a general class of coefficients $Q$, the magnitude of the error term $\epsilon_M(x)$ for large $x$ decreases as $M$ increases. This feature of $\epsilon_M(x)$ was then exploited in [**3**] for the case where $Q(x)=q(x)-\lambda$ and (1·2) becomes the usual Sturm–Liouville equation with spectral parameter $\lambda$. The smallness of $\epsilon_M(x)$ for a suitable choice of $M$ (such as $M=6$) leads to an efficient numerical algorithm for estimating the Titchmarsh–Weyl function $m(\lambda)$ with precise global error bounds. In [**3**], the case where $q(x)=-x^\alpha$ $(0<\alpha\leqslant 2)$ and $\operatorname{Re}\lambda\geqslant -1$ was considered in detail.

In this paper, we develop these ideas for higher-order differential equations. Thus we consider the generalization of (1·1) for the $n$th order equation

$$y^{(n)}(x)-Q(x)\,y(x)=0 \tag{1·3}$$

again with improving estimates on $\epsilon_M$ as $M$ increases. In the case where $n$ is even, $n=2\nu$, and $Q(x)=(-1)^\nu\{\lambda-q(x)\}$, we have a $\nu\times\nu$ spectral matrix $(m_{ij}(\lambda))$ which corresponds to the Titchmarsh–Weyl function $m(\lambda)$ [**14**], and we can again apply our estimates for $\epsilon_M$ to obtain numerical estimates for the spectral matrix.

There are however certain difficulties which arise when $n>2$ and which were not present for the second-order equation (1·2). The first is that, when $n>2$, it is no

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longer possible to diagonalize the $n \times n$ matrices in the associated first-order systems in the same explicit way as when $n = 2$. We overcome this difficulty by adopting an approximate diagonalization process and this approach is discussed in Sections 2 and 3. Secondly, this approximate procedure necessarily involves differential systems whose coefficient matrices contain a greater number of terms than when $n = 2$, and we have to develop a new algorithm for generating and collating these terms. These matters are introduced in Sections 4 and 5. Then in Section 6, we develop a computational algorithm to perform the repeated diagonalization. The estimation of error terms leading to $\epsilon_M$ presents fewer difficulties and it is also dealt with in Section 6. The application to the spectral matrix $(m_{ij}(\lambda))$ is naturally les simple than when $n = 2$ because the underlying spectral theory involves several $L^2(0, \infty)$ solutions of the differential equation rather than just one such solution. We cover this application in Sections 7 and 8 with special reference to the example $q(x) = -x^\alpha$ $(\alpha > 0)$. In Section 9 we are able to give independent confirmation of our results when $\alpha = 1$ in terms of the higher-order Airy equation. Finally, in Section 10 we indicate possible estensions of our work and, in both Sections 8 and 10, we comment on the effectiveness of our methods as compared with the recent alternative approach of Bennewitz *et al.* [**2**].

## 2. *Diagonalization in differential systems*

In this section we introduce the theoretical basis for estimating and improving error terms in the solution of differential systems. These error terms give rise to $\epsilon_M$ in (2·1) and in the corresponding formulae for (1·3) (see 3·14) in the next section). The main components of the discussion are covered in the three subsections (a)–(c) below, and we frame it in terms of the system

$$Z'(x) = x^\beta \{D + O(x^{-\gamma})\} Z(x), \tag{2·1}$$

where $D$ is a constant diagonal $n \times n$ matrix,

$$D = \mathrm{dg}\,(d_1, \ldots, d_n)$$

with distinct $d_k$ and the $O$-term refers to $x \to \infty$. Also, $\beta > 0$ and $\gamma > 0$. If, in addition, $\beta - \gamma < -1$, (2·1) has the standard Levinson form [**20**] [**11**, section 1·3]

$$Z' = (\Lambda + R) Z \tag{2·2}$$

in which $\Lambda$ is diagonal and $R$ is $L(a, \infty)$, and the Levinson asymptotic theorem [**11**, theorem 1·3·1] states that there are solutions $Z_k (1 \leqslant k \leqslant n)$ of (2·1) such that

$$Z_k(x) = (e_k + \eta_k) \exp\left( \int_a^x t^\beta d_k \, dt \right), \tag{2·3}$$

where $e_k$ is the unit coordinate vector in the $k$-direction and $\eta_k \to 0$ as $x \to \infty$. The size of $\eta_k$ is related to the size of $x^{\beta-\gamma}$ as $x \to \infty$ in a manner to be made precise in Section 3.

(*a*) *Exact diagonalization.* We first consider the effect of expressing the coefficient matrix in (2·1) in its diagonal form and, as a start, we suppose that the O-term is simply $x^{-\gamma} C$, where $C$ is a constant. Thus we write

$$T^{-1}(D + x^{-\gamma} C)\, T = D_1, \tag{2·4}$$

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where $D_1$ is the diagonal matrix formed by the eigenvalues of $D+x^{-\gamma}C$ and $T$ is the approximate identity matrix formed by the eigenvectors. Then

$$D_1 = D+O(x^{-\gamma}), \quad T = I+O(x^{-\gamma}), \quad T' = O(x^{-\gamma-1})$$

as $x \to \infty$. The transformation

$$Z = TW \tag{2·5}$$

therefore takes (2·1) into

$$W' = x^{\beta}(D_1 - x^{-\beta}T^{-1}T')\,W = x^{\beta}\{D_1 + O(x^{-\beta-\gamma-1})\}\,W. \tag{2·6}$$

Hence the effect of the transformation (2·5) is to replace the perturbation $x^{-\gamma}$ in (2·1) by one of smaller magnitude $x^{-\beta-\gamma-1}$ in (2·6)

Even though (2·6) does not have quite as simple a form as we specified in (2·1), the argument which leads from (2·1) to (2·6) can again be applied to (2·6) to yield a sequence of systems

$$W'_m = x^{\beta}(D_m + R_m)\,W_m \tag{2·7}$$

with approximately constant diagonal matrices $D_m$ and perturbations $R_m$ of magnitude $x^{-m(\beta+1)-\gamma}(m = 1, 2, \dots)$. The Levinson formula (2·3) can be applied to any system in the sequence, and the term $\eta_k$ will have a corresponding order of magnitude. The transformation back to the original system (2·1) via the sequence of equations such as (2·5) thus gives successively more accurate asymptotic representations of the solutions of (2·1).

The details of this process were given in [**3**, sections 2–3] for the case where (2·1) arises from (1·2) and all the matrices are $2 \times 2$. These details depended on the explicit knowledge of all necessary eigenvalues and eigenvectors in equations such as (2·4). When $n > 2$, however, such explicit knowledge is not available in (2·4). In this paper, we overcome this difficulty by modifying (2·4) and considering instead an approximate diagonalization process which is based on the one introduced by Eastham [**9**] [**11**, section 1·7].

(*b*) *Approximate diagonalization.* The matrix $T$ in (2·5) has the form $T = I+P$, where $P = O(x^{-\gamma})$, and the idea now is to modify (2·5) to

$$Z = (I+P)\,W \tag{2·8}$$

with a different, but explicit $P$. It follows from [**11**, (1·7·2) and (1·6·13)] that (2·8) represents an approximation to (2·5) if $P$ is defined by

$$PD - DP = x^{-\gamma}(C - \operatorname{dg} C) \tag{2·9}$$

with $\operatorname{dg} P = 0$. Thus the entries $p_{ij}$ in $P$ are defined by

$$p_{ij} = x^{-\gamma}c_{ij}/(d_j - d_i) \quad (i \neq j). \tag{2·10}$$

By (2·8) and (2·9), we obtain in place of (2·6)

$$\begin{aligned} W' &= x^{\beta}\{D + x^{-\gamma}(I+P)^{-1}(CP + \operatorname{dg} C) - x^{-\beta}(I+P)^{-1}P'\}\,W \\ &= x^{\beta}\{D_1 + x^{-\gamma}(I+P)^{-1}(CP - P\operatorname{dg} C) - x^{-\beta}(I+P)^{-1}P'\}\,W. \end{aligned} \tag{2·11}$$

Here

$$D_1 = D + x^{-\gamma}\operatorname{dg} C \tag{2·12}$$

and, by (2·10), the other two groups of terms are respectively $O(x^{-2\gamma})$ and $O(x^{-\beta-\gamma-1})$, of which the latter dominates if $\gamma > \beta+1$. We note that (2·11) contains more terms

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than (2·6), but this is the price to be paid for having explicit terms derived from (2·10).

(*c*) *Further approximation.* Repetition of the process (2·8)–(2·11), but with (2·11) as the starting point, involves the diagonal entries of $D_1$ in place of $d_j$ and $d_i$ in (2·10). Thus powers of $x$ appear increasingly in the denominators of the $P$-matrices. This causes problems when we seek to develop computing and numerical procedures for implementing the repeated transformations, particularly because repeated differentiation of such matrices is involved, as indicated by the appearance of $P'$ in (2·11). Accordingly, we shall retain the original constant entries $d_j$ and $d_i$ in the denominators as we go through the process. This further approximation adds new terms to the coefficient matrices $\{\dots\}$ in the sequence of systems corresponding to (2·11). It is this last method that we adopt in this paper and, after these introductory remarks, we defer further details to Section 4 where we deal with the actual system (2·1) which arises from (1·3).

## 3. *Asymptotic formulae for solutions*

The dominant form of the solutions of (1·3) for large $x$ is known subject to suitable conditions on $Q$ [**11** section 2·9]. Our aim here is to obtain an explicit estimate for the error terms in the asymptotic formulae, which is suitable for our purposes in Sections 4–6. We begin with the system formulation

$$Z' = (\Lambda + R)\, Z \tag{3·1}$$

of (1·3) which is given in [**11**, section 2·9]. Here

$$\Lambda = Q^{1/n}\, \mathrm{dg}\,(\omega_1, \dots, \omega_n), \tag{3·2}$$

where

$$\omega_k = \exp\{2(k-1)\,\pi i/n\}$$

are the $n$-th roots of unity, and

$$R = -\Omega^{-1}\Lambda_1\,\Omega, \tag{3·3}$$

where

$$\Lambda_1 = n^{-1}(Q'/Q)\,\mathrm{dg}\,(0, 1, \dots, n-1), \tag{3·4}$$

while $\Omega$ and $\Omega^{-1}$ have $(j,k)$ entries $\omega_k^{j-1}$ and $n^{-1}\omega_j^{-(k-1)}$ respectively. The connection between $Z$ and $y$ in (3·1) and (1·3) is

$$Y = \{\mathrm{dg}\,(1, Q^{1/n}, Q^{2/n}, \dots, Q^{(n-1)/n})\}\,\Omega Z, \tag{3·5}$$

where $Y$ has components $y, y', \dots, y^{(n-1)}$. It follows from (3·2)–(3·4) that (3·1) can be written in the form

$$Z' = Q^{1/n}(D + Q'Q^{-1-1/n}C)\, Z, \tag{3·6}$$

where $C$ is constant and

$$D = \mathrm{dg}\,(\omega_1, \dots, \omega_n). \tag{3·7}$$

In the case where $Q$ and its derivative sufficiently resemble $x^\alpha$ $(\alpha > 0)$ and its derivatives, the system (3·6) essentially has the form (2·1) with $\gamma = 1 + \alpha/n$, and the ideas in Section 2 for improving the error term apply. At this point, we note that the diagonal entries in $C$ are all $-(n-1)(2n)^{-1}$ [**11**, (2·9·25)] and this, together with (2·12), governs our definition of $D_M$ and $D_m$ in (3·10) and (4·4) below.

The sequence of transformations to be defined in Section 4 takes (3·6) into the form

$$Z'_M = Q^{1/n}(D_M + R_M)\, Z_M, \tag{3·8}$$

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where
$$Z = \left\{\prod_1^{M-1}(I+P_m)\right\} Z_M = (I+P)\,Z_M, \tag{3·9}$$

$$D_M = D-(n-1)\,(2n)^{-1}\,Q'Q^{-1-1/n}I+\Delta_M \tag{3·10}$$

and $R_M \in L(X,\infty)$. Also $P(x)$ and $\Delta_M(x)$ are both $o(1)$ as $x\to\infty$. We can now state and prove a lemma which gives the asymptotic form of the solutions of (1·3), incorporating an explicit estimate of the error term derived from a knowledge of $R_M$. In the lemma we write $P=(p_{ij})$ and $\Delta_M = \mathrm{dg}\,(\delta_{1M},\dots,\delta_{nM})$.

LEMMA 3·1. *Let $M\,(\geqslant 2)$ be an integer and let $D_M$, $R_M$ and $P$ be as in* (3·8)–(3·10). *In some interval $[X,\infty)$, let*

$$\mathrm{Re}\,\{(\omega_j-\omega_k+\delta_{jM}-\delta_{kM})\,Q^{1/n}\} \quad (1\leqslant j,k\leqslant n) \tag{3·11}$$

*have constant sign (either $\geqslant 0$ or $\leqslant 0$), with*

$$\left|\int_X^\infty \mathrm{Re}\,\{(\omega_j-\omega_k+\delta_{jM}-\delta_{kM})\,Q^{1/n}\}\,dt\right| = \infty \tag{3·12}$$

*for $j\neq k$. Also, let*

$$\int_X^\infty |Q^{1/n}(t)\,R_M(t)\,dt| < \infty. \tag{3·13}$$

*Then, for $1\leqslant k\leqslant n$ and $1\leqslant r\leqslant n$,* (1·3) *has solutions $y_k$ such that*

$$y_k^{(r-1)} = Q^{-(n+1-2r)/2n}\left\{\omega_k^{r-1}+\sum_{j=1}^n \omega_j^{r-1}\left(\eta_j+p_{jk}+\sum_{l=1}^n p_{jl}\,\eta_l\right)\right\} \times \exp\left(\int_X^x Q^{1/n}(t)\,\{\omega_k+\delta_{kM}(t)\}\,dt\right), \tag{3·14}$$

*where, in $[X,\infty)$, the $\eta_j$ $(1\leqslant j\leqslant n)$ satisfy the estimate*

$$|\eta_j(x)| \leqslant \int_X^\infty |Q^{1/n}(t)|\,\|R_M(t)\|\,dt \Big/ \left(1-n\int_X^\infty |Q^{1/n}(t)|\,\|R_M(t)\|\,dt\right) \tag{3.15}$$

*with $\|R_M\| = \max|r_{ijM}|$ $(1\leqslant j,k\leqslant n)$ in terms of the entries in $R_M$.*

*Proof.* By (3·11) and (3·13), we can apply the Levinson theorem [**11**, theorem 1·3·1] to the system (3·8), and then transform back to $Y$ via (3·9) and (3·5) to obtain vectors $Y$ with the form

$$Y = \mathrm{dg}\,(1,Q^{1/n},\dots,Q^{(n-1)/n})\,\Omega(I+P)\,(e_k+u) \times \exp\left(\int_X^x [Q^{1/n}\{\omega_k+\delta_{kM}\}-(n-1)\,(2n)^{-1}\,(Q'/Q)]\,(t)\,dt\right), \tag{3·16}$$

where $u=o(1)$ and we have used (3·10). Let $u$ have components $\eta_j$ $(1\leqslant j\leqslant n)$. Then (3·14) follows from (3·16) on taking the $r$th component on each side.

It remains to establish (3·15) and, to do this, we proceed as in [**11**, (1·4·23) and (1·4·13)]. It follows from (3·11) and (3·12) that, in the notation of [**11**, (1·4·13)], the non-zero entries of $\Phi_1(x)\,\Phi^{-1}(t)$ and $\Phi_2(x)\,\Phi^{-1}(t)$ are all $\leqslant 1$ in modulus. Hence [**11**, (1·4·13)] (with $a=X$ here) gives

$$|\eta_j(x)| \leqslant \int_X^\infty \left(|Q^{1/n}r_{jkM}|+\sum_{l=1}^n |Q^{1/n}r_{jlM}\,\eta_l|\right)dt.$$

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Thus, if $H = \max|\eta_j|$ $(X \leqslant x < \infty, 1 \leqslant j \leqslant n)$, we obtain

$$H \leqslant \int_X^\infty (|Q^{1/n}|\,\|R_M\| + H_n|Q^{1/n}|\,\|R_M\|)\,dt.$$

Hence

$$H \leqslant \int_X^\infty |Q^{1/n}|\,\|R_M\|\,dt \Big/ \left(1 - n\int_X^\infty |Q^{1/n}|\,\|R_M\|\,dt\right),$$

and (3·15) follows.

## 4. *The sequence of transformations*

In this section we define the transformations

$$Z_m = (I + P_m)\,Z_{m+1} \quad (1 \leqslant m \leqslant M-1) \tag{4·1}$$

which lead from (3·6) to (3·8) in the manner introduced in Section 2(*c*). A typical sytem in the procss is

$$Z'_m = Q^{1/n}(D_m + R_m)\,Z_m \tag{4·2}$$

with (3·6) being the case $m = 1$. In (3·6), we emphasize the role of the diagonal terms in $C$ by taking these terms over to $D$ as in (3·10). Thus we define

$$D_1 = D + \tfrac{1}{2}(n-1)\,pI, \quad R_1 = Q'Q^{-1-1/n}(C - \mathrm{dg}\,C) \tag{4·3}$$

with $D$ as in (3·7) and $p = (Q^{-1/n})' = -n^{-1}Q'Q^{-1-1/n}$. Then, again as in (3·10), we write

$$D_m = D_1 + \Delta_m \quad (m \geqslant 2). \tag{4·4}$$

Now, as indicated by (2·11), $R_m$ will contain terms of different orders of magnitude as $x \to \infty$, and we wish to identify these terms according to their size. Hence we write

$$R_m = V_m + E_m = V_{1m} + V_{2m} + \ldots + V_{\mu m} + E_m, \tag{4·5}$$

where

$$V_{km} = o(V_{jm}) \quad (x \to \infty, k > j) \tag{4·6}$$

and

$$E_m = o(V_{\mu m}) \quad (x \to \infty). \tag{4·7}$$

Here $E_m$ represents terms which are already of the accuracy that we require in (3·15), while the $V_{jm}$ represent terms which are not of that accuracy and which have to be replaced by smaller-order terms as we go through the transformation process in the manner discussed in Section 2. Also, as in the case of (4·3), we arrange that

$$\mathrm{dg}\,V_{1m} = 0. \tag{4·8}$$

To discuss a typical step in the process leading to (3·8), we substitute (4·1) into (4·2) to obtain

$$\begin{aligned}(I + P_m)\,Z'_{m+1} + P'_m\,Z_{m+1} &= Q^{1/n}(D_m + R_m)(I + P_m)\,Z_{m+1}\\ &= Q^{1/n}\{(I + P_m)\,D_m + D_m P_m - P_m D_m + V_{1m} + V_{1m}P_m + (R_m - V_{1m})(I + P_m)\}\,Z_{m+1}.\end{aligned} \tag{4·9}$$

Now we define $P_m$ by

$$P_m D - DP_m = V_{1m} \tag{4·10}$$

with $\mathrm{dg}\,P_m = 0$, this definition being consistent in the diagonal entries because of (4·8). Thus the entries $p_{ijm}$ in $P_m$ are defined by

$$p_{ijm} = v_{ij1m}/(\omega_j - \omega_i), \tag{4·11}$$

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again as indicated by (2·9), (2·10) and Section 2(*c*). It follows from (4·4) and (4·10) that in (4·9) we have

$$D_m P_m - P_m D_m + V_{1m} = \Delta_m P_m - P_m \Delta_m = T_m, \tag{4·12}$$

say. Hence, so far, (4·9) gives

$$Z'_{m+1} = Q^{1/n}\{D_m + (I+P_m)^{-1}(-Q^{-1/n}P'_m + T_m + V_{1m}P_m + (R_m - V_{1m})(I+P_m))\}Z_{m+1}. \tag{4·13}$$

We wish to show that this can be expressed as

$$Z'_{m+1} = Q^{1/n}(D_{m+1} + R_{m+1})Z_{m+1}, \tag{4·14}$$

where $R_{M+1}$ has a similar form to (4·5):

$$R_{m+1} = V_{m+1} + E_{m+1} = V_{1,m+1} + \ldots + V_{\mu,m+1} + E_{m+1}, \tag{4·15}$$

but with a different $\mu$, and where the $V_{j,m+1}$ can be obtained constructively from the $V_{jm}$. Also, as in (4·8), we shall arrange that

$$\mathrm{dg}\, V_{1,m+1} = 0. \tag{4·16}$$

We establish (4·15) by writing

$$(I+P_m)^{-1} = I - P_m + P_m^2 - \ldots + (-1)^\nu P_m^\nu + (-1)^{\nu+1}(I+P_m)^{-1}P_m^{\nu+1}. \tag{4·17}$$

Here $\nu$ is chosen so that the product

$$(I+P_m)^{-1}P_m^{\nu+1}V_{jm},$$

which occurs in (4·13), has a sufficiently small order of magnitude to be included with $E_m$ and form part of $E_{m+1}$. Thus $\nu$ will differ for different $j$, and similarly for the other terms in (4·13). We now group together terms of the same order of magnitude and denote the dominant term by $S_{m+1}$. We then obtain (4·15) (with $S_{m+1}$ in place of $V_{1,m+1}$), where $E_{m+1}$ has the same order of magnitude as $E_m$ and, by (4·11), $S_{m+1}$ and the $V_{j,m+1}$ are known explicitly in terms of the $V_{jm}$. We complete the derivation of (4·14) and (4·15), in which (4·16) holds, by defining

$$D_{m+1} = D_m + \mathrm{dg}\, S_{m+1} \tag{4·18}$$

and

$$V_{1,m+1} = S_{m+1} - \mathrm{dg}\, S_{m+1}.$$

In the next two sections, we deal with the question of developing an algorithm, to be implemented in the symbolic algebra system *Mathematica*, for determining the $V_{jm}(m = 1, 2, \ldots)$ and estimating the $E_m$.

## 5. *The basis of the algorithm*

The details of the procedure based on (4·5)–(4·18) depend on the nature of $Q$. In this section we assume that

$$Q(x) \sim (\text{const.})\, x^\alpha \quad (x \to \infty), \tag{5·1}$$

where $\alpha > 0$, and that differentiation can be carried out in the sense that

$$Q^{(r)}(x) = (\text{const.})\, x^{\alpha - r}\{1 + o(1)\}. \tag{5·2}$$

At the end of the paper, we indicate the modifications which are made to accommodate other types of $Q$.

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We start the detailed examination of (4·5)–(4·7) with the cases $m = 1$ and 2. When $m = 1$, (4·2) is (3·6) and, as in (4·3), we have

$$D_1 = D + \tfrac{1}{2}(n-1)\,pI, \quad R_1 = Q'Q^{-1-1/n}(C - \mathrm{dg}\,C) = O(x^{-a}), \tag{5·3}$$

by (5·1) and (5·2), where

$$a = 1 + \alpha/n. \tag{5·4}$$

So far, we have only $\mu = 1$ and $E_1 = 0$ in (4·5). Then (4·13) is simply

$$Z_2' = Q^{1/n}\{D_1 + (I + P_1)^{-1} S_z\} Z_2, \tag{5·5}$$

where

$$S_2 = -Q^{-1/n} P_1' + R_1 P_1. \tag{5·6}$$

By (4·11) and (5·1)–(5·3), we have

$$P_1 = O(x^{-a}), \quad S_2 = O(x^{-2a}). \tag{5·7}$$

For the inverse matrix in (5·5), we use (4·17) and, at this point, we specify the accuracy to be represented by the $E_m$ in (4·5). We require

$$E_m = O(x^{-(N+2)a}) \tag{5·8}$$

for all $m$ and a fixed integer $N \geqslant 0$. Thus the process leading to (3·8) ends when (4·5) reduces to

$$R_M = E_M. \tag{5·9}$$

Then by (4·17), we have

$$(I + P_1)^{-1} S_2 = \left( \sum_{j=1}^{N} (-1)^{j-1} P_1^{j-1} \right) S_2 + (-1)^N (I + P_1)^{-1} P_1^N S_2.$$

Thus (5·5) is the case $m = 2$ of (4·2), where (4·5) holds with $\mu = N$, $V_{j2} = (-1)^{j-1} P_1^{j-1} S_2$ $(2 \leqslant j \leqslant N)$ and

$$E_2 = (-1)^N (I + P_1)^{-1} P_1^N S_2.$$

Also, as in (4·18),

$$D_2 = D_1 + \mathrm{dg}\,S_2, \quad V_{12} = S_2 - \mathrm{dg}\,S_2.$$

We note that, by (5·7),

$$V_{j2} = O(x^{-(j+1)a}), \quad E_2 = O(x^{-(N+2)a}) \tag{5·10}$$

and, by (4·4),

$$\Delta_2 = \mathrm{dg}\,S_2 = O(x^{-2a}).$$

Then, since $\Delta_m$ $(m \geqslant 3)$ is obtained from (4·18) by adding successively smaller-order terms to $\Delta_2$, we have

$$\Delta_m = O(x^{-2a}) \tag{5·11}$$

for all $m$.

We move on to general $m$ in (4·5). An easy induction argument starting from (5·3) and (5·10), and based on (4·11) and (4·17), shows that

$$V_{jm} = O(x^{-(m+j-1)a}). \tag{5·12}$$

Then by (5·1) and (5·11), it follows from (4·11) and (4·12) that

$$P_m = O(x^{-m}), \quad Q^{-1/n} P_m' = O(x^{-(m+1)a}), \quad T_m = O(x^{-(m+2)a}). \tag{5·13}$$

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It now follows from (4·5), (5·12) and (5·13) that, in (4·14) and (4·15),

$$V_{1,m+1} = -Q^{-1/n}P'_m + (V_{2m} - \mathrm{dg}\, V_{2m}) \tag{5·14}$$

and then (5·14) is used in (4·11) to define $P_{m+1}$. A further consequence of (4·5) and (5·12) is that (5·9) is achieved when

$$M = N+2. \tag{5·15}$$

It is not diffult to check that the order relations (5·12) and (5·13) are in fact exact, and we can describe (5·12) by saying that $V_{jm}$ has exact order $m+j-1$, and similarly for (5·13). The grouping together of terms of the same order is the basis of the algorithm which we go on to describe in more detail now.

## 6. *A symbolic algorithm for the computation of solutions*

We can now use the ideas in Section 5 to discuss the development of a computational algorithm for computing the solutions of (1·3) over an interval $[X, \infty)$, subject to (5·1) (5·2). The algorithm is implemented in the symbolic algebra system *Mathematica* and we use the notation in Sections 3–5 to denote the symbolic objects that we need. The algorithm computes estimates for $n$ linearly independent solutions of (1·3), and for the derivatives, and it is structured in three distinct stages. In the first stage, we shall not make any assumptions about the order of the differential equation while, for reasons of clarity, in the second and third stages our discussion is focused on the case $n = 4$ and more particularly on the equation

$$y^{(4)} - x^{\alpha}y = \lambda y \quad (X \leqslant x < \infty), \tag{6·1}$$

where $X > 0$ and $\alpha > 0$, this equation being covered by (5·1) and (5·2).

We recall that the discussion in Sections 4–5 of this paper shows how the system

$$Z'_m = Q^{1/n}(D_m + V_m + E_m)\, Z_m \tag{6·2}$$

is transformed into

$$Z'_{m+1} = Q^{1/n}(D_{m+1} + V_{m+1} + E_{m+1})\, Z_{m+1} \tag{6·3}$$

by the mapping

$$Z_m = (I + P_m)\, Z_{m+1}. \tag{6·4}$$

Here $P_m$, $D_m$ and $V_m$ are defined in (4·11), (4·18), (4·5) and (4·8), where $V_{jm}$ has exact order $m+j-1$ as described at the end of Section 5. We now restate some of the features of this discussion in a suitable form for implementation in our algorithm.

First, the number $M$ which appears in (3·8) and (5·9) is determined by the accuracy of our working which, by (5·8) and (5·15), can now be stated as

$$E_m = O(x^{-Ma}) (1 \leqslant m \leqslant M). \tag{6·5}$$

Then, by (5·12), we have $\mu = M - m$ in (4·5). Next, examining the use of (4·17) in (4·13), we denote by $U$ any one of the terms in (4·13) on which the inverse acts, excepting $E_m$. Thus

$$U \in \{-Q^{-1/n}P'_m, T_m, V_{1m}P_m, V_{jm}, V_{jm}P_m \quad (2 \leqslant j \leqslant M-m)\}. \tag{6·6}$$

For each $U$, the integer $\nu$ in (4·17) is chosen so that $P_m^{\nu+1}U$ has sufficiently small order of magnitude to satisfy (6·5). Since the order of $U$ is known from (5·12) and (5·13),

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the computation of $\nu$ and the grouping of terms $(-1)^r P_m^r U$ $(0 \leqslant r \leqslant \nu)$ of the same order can be performed for each $U$ and $r$.

By (4·5), the error term $E_m$ appears in (4·13) in the form

$$A_m E_m (I+P_m),$$

where the symbol $A_m$ stands for $(I+P_m)^{-1}$. This is taken as an initial definition of $E_{m+1}$ which is then updated as (4·17) is used for each $U$, to yield the final $E_{m+1}$ in (4·15).

This discussion leads to the following algorithm, based on (4·11) and (4·17), for computing the $V_{jm}$ and $S_m$ – and hence the $D_m$ and $V_m$ – in Sections 4 and 5.

Algorithm 6·1. (1) *First input $M$ to fix both the number of iterations required for* (3·8) *and the order* (6·5) *of $E_M$.*

(2) *Start with $D_1$ and $V_1$, and put $E_1 = 0$.*

(3) *For $m = 1$ to $M-1$, $E_{m+1} = A_m E_m (I+P_m)$.*

(4) *For each $U$ in* (6·6), *determined $\nu$, the number needed in* (4·17).

(5) *Update error term, i.e. $E_{m+1} = E_{m+1} + (-1)^\nu A_m P_m^{\nu+1} U$.*

(6) *For $r = 0$ to $\nu$, determine the exact order $\rho = mr + (\text{order of } U)$ of $P_m^r U$.*

(7) *Update $V_{\rho-m,\,m+1} = V_{\rho-m,\,m+1} + (-1)^r P_m^r U$ $(\rho - m \geqslant 2)$.*

*Then, as in* (5·14),

$$S_{m+1} = -Q^{-1/n} P'_m + V_{2m}$$

*and*

$$V_{1,\,m+1} = S_{m+1} - \operatorname{dg} S_{m+1}.$$

At any stage in the algorithm, $S_{m+1}$ depends on the terms $D_j, P_j, P'_j$ and $V_j$ $(1 \leqslant j \leqslant m)$. However, simplifications can be made by retaining earlier terms $S_j$ where possible. This reduces the number of terms in the computation of $S_{m+1}$ with consequent economy in the algorithm. We illustrate this point by giving the results for $S_3$ and $S_4$ which are first obtained in terms of $V_1, V_2, P_1$ etc, and then the previously computed definition of $S_2$ is used dynamically to simplify the expressions for $S_3$ and $S_4$. Thus we have

$$S_2 = -\frac{P'_1}{Q^{\frac{1}{n}}} + V_1 P_1 \quad \text{(as in (5·6))}$$

$$S_3 = -\frac{P'_2}{Q^{\frac{1}{n}}} + T_1 - P_1 S_2$$

$$S_4 = -\frac{P'_3}{Q^{\frac{1}{n}}} + T_2 - P_1 T_1 + V_2 P_2 + P_1^2 S_2.$$

We also give the error term $E_5$ as an example:

$$\begin{aligned} E_5 = {} & A_4 A_3 A_2 A_1 \{P_1^2 T_1 - P_1^3 S_2\} (I+P_2)(I+P_3)(I+P_4) \\ & + A_4 A_3 A_2 \{(-P_1 T_1 + P_1^2 S_2 - P_1 S_2 + T_1) P_2 \\ & - P_2 (S_2 - P_1 T_1 + P_1^2 S_2 + T_2 + V_2 P_2)\} (I+P_3)(I+P_4) \\ & + A_4 A_3 \{T_3 - P_3 S_2 + V_3 P_3 + (-P_1 T_1 + P_1^2 S_2 + V_2 P_2 + T_2) P_3\} (I+P_4) \\ & + A_4 \left( -\frac{P'_4}{Q^{\frac{1}{n}}} + T_4 + V_4 P_4 \right). \end{aligned}$$

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Table 1. *Time in seconds for computing expressions $S_m$ and $E_m$*

| $m$ | Duration in seconds |
|---|---|
| 4 | 1·6167 |
| 6 | 7·5000 |
| 7 | 22·4167 |
| 8 | 61·9833 |

The expression

$$S_6 = -Q^{-\frac{1}{n}}P_5' + T_4 + (-P_1 T_1 + P_1^2 S_2) P_2 \\ -P_2(-P_1 T_1 + V_2 P_2 + P_1^2 S_2 + T_2) - P_1^3 T_1 + P_1^4 S_2 + V_3 P_3$$

which we use later in our examples, has an associated error term $E_6$ with over 250 components. The numbers of components in $S_8$ and $E_8$ are about 60 and 700 respectively. This complexity indicates that the computation is intractable by hand, and that a symbolic algebra system is the only way to generate the recurrences. The algorithm is however quite cheap to compute, and we give some sample times in Table 1.

At this stage, the algorithm involves nothing more than a series of recurrence formulae in terms of objects which satisfy non-commutative multiplication and certain order relations. When we wish to go further and apply the algorithm to a specific equation (1·3), we need to express the recurrence formulae in terms of $n \times n$ matrices, and in the next stage of the algorithm, we focus on $n = 4$. In this case (3·7) becomes

$$D = \mathrm{dg}\,(1, i, -1, -i)$$

and, in (4·3),

$$p = -\tfrac{1}{4}Q'Q^{-5/4}. \tag{6·7}$$

Also, it is easily verified from (3·3) and (4·3) that $V_1 (= R_1)$ has the form to be stated now.

Algorithm 6·2. *Starting with initial matrices*

$$D_1 = D + \tfrac{3}{2}pI,$$

$$V_1 = -\tfrac{1}{2}p \begin{pmatrix} 0 & 1+i & 1 & 1-i \\ 1-i & 0 & 1+i & 1 \\ 1 & 1-i & 0 & 1+i \\ 1+i & 1 & 1-i & 0 \end{pmatrix},$$

*and $E_1 = 0$, the expressions $S_2, \ldots, S_{M-1}$ generated in Algorithm 6·1 are evaluated in order. These are then used in turn to generate the $4 \times 4$ matrices $D_2, \ldots, D_{m-1}$, $V_2, \ldots, V_{M-1}, P_2, \ldots, P_{M-1}, P_2', \ldots, P_{M-1}'$.*

We note that the process stops at $M-1$ because (5·9) implies that $D_M = D_{M-1}$ and $V_M = 0$. In Algorithm 6·2, we assume only that $p$ and $Q$ are sufficiently smooth functions related by (6·7) and

$$Q'' = -4Q^{\frac{5}{4}}p' + 20p^2Q^{\frac{3}{2}}. \tag{6.8}$$

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Table 2. *Time in seconds for computing matrices* $S_m$

| $m$ | Duration in seconds |
|---|---|
| 4 | 74·6167 |
| 6 | 904·24 |
| 7 | — |

This equation is used to express higher order derivatives of $Q$ in terms of those of $p$.

There are several severe computational problems contained in this seemingly simple process of matrix multiplication and substitution. Although all the operations needed are to be found in the Mathematica system, the use of the Substitute command in Mathematica requires an inordinate amount of computational effort, and therefore it is necessary to consider what substitutions and simplifications are best used at each stage of the algorithm. The relationships in (6·7) and (6·8) have been found most useful in simplifying the expressions produced by this part of the algorithm. The main problem however, manifested by long computing times, lies in the exponential growth of the number of terms in the elements of the matrices $S_m$. For example, each of the elements of $S_6$ consists of a sum of over one thousand terms, each of which is a product of several distinct objects. A consequence of this complexity is that, as $m$ increases, the amount of computational effort required to perform the calculations increases exponentially. The time in cpu seconds needed to compute $S_4$ and $S_6$ on a SPARC 10 workstation, is given in Table 2. The — indicates that it has not been possible to complete the computation within a reasonable time. This is because of the limitations in the size of memory and cpu speed that we have available.

The final stage of the algorithm deals with the remaining matter of obtaining an explicit upper bound for the norm $\|E_m\|$ of $E_m$ which adds precision to the order estimate (6·5) and which can be used in (3·15) when $m = M$. We use the sup norm, for which the triangle and Cauchy inequalities are

$$\|A+B\| \leqslant \|A\|+\|B\|, \quad \|AB\| \leqslant 4\|A\|\,\|B\|$$

in our case of $4\times 4$ matrices. For the inverse matrix $A_m = (I+P_m)^{-1}$, we have from the geometric series

$$\|A_m\| \leqslant 1+\sum_{r=1}^{\infty}\|P_m^r\| \leqslant 1+\sum_{r=1}^{\infty}4^{r-1}\|P_m\|^r$$

and hence

$$\|A_m\| \leqslant 1+\|P_m\|/(1-4\|P_m\|) \tag{6·9}$$

provided that $\|P_m\| < 1/4$.

There is one other point to mention before discussing this final stage of the algorithm, and this is prompted by the fact that the reciprocal of $Q$ occurs throughout the process in Algorithms 6·1 and 6·2. In order to estimate this reciprocal, we require a lower bound for $Q$ in the relevant $x$-interval $[X, \infty)$. Thus, in addition to (5·1) and (5·2), we require that

$$|Q(x)| \geqslant k^{-1}x^{\alpha} \quad (X \leqslant x < \infty) \tag{6·10}$$

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Table 3. *Time in seconds for computing norms where* $k = \frac{11}{10}$ *and* $\alpha = 1$

| | Durations in seconds | | |
|---|---|---|---|
| $m$ | $S_m$, $R_m$, $P_m$, $A_m$ norms | $T_m$ norms | $P'_m$ norms |
| 4 | 167·833 | 148·25 | 241·33 |
| 6 | 1159·5 | 1446·2 | 2216·25 |
| 7 | 3297·95 | — | — |

for some constant $k > 1$. In (6·1) itself, we have $Q(x) = \lambda + x^\alpha$, and we shall consider $\lambda$ in the half plane

$$\operatorname{Re}\lambda \geqslant -1. \tag{6·11}$$

Thus $|Q(x)| \geqslant |\operatorname{Re}\lambda + x^\alpha| \geqslant (1 - X^{-\alpha})\, x^\alpha$ provided that $X > 1$. Thus (6·10) holds with

$$k = (1 - X^{-\alpha})^{-1}.$$

Algorithm 6·3. *Compute the sup. norm of each matrix in* $E_m$, *using* (6·9) *for the inverse matrices. Next apply the triangle and Cauchy inequalities to obtain an upper bound for the sup. norm of* $E_m$ *itself.*

The terms that we encounter in computing the matrix norms involve $p$ and its derivatives. In order to obtain an upper bound for the $k$th derivative of $p(x)$, we first use

$$Q(x) = \lambda + x^\alpha$$

and (6·8) to compute a symbolic expression of $p^{(k)}$. We then use the inequality (6·10) to compute bounds for $|p^{(k)}(x)|$. In obtaining this estimate every element of every matrix which occurs in the error term $E_M$ must be examined. The triangle and Cauchy inequalities are applied to each element and the bounds for $|Q|$ and $|p^{(r)}|$ are substituted with $k \geqslant (1 - X^{-\alpha})^{-1}$ and the specific values of $X$ and $\alpha$ under consideration. This enables the sup. norm of each matrix to be computed at the point $X$ and a precise upper bound $\epsilon(X)$ for the error in the solutions determined. Again the amount of computational effort needed is exponentially increasing with the requested number of iterations. In Table 3 we show, where possible, the amount of cpu time needed to compute these norm estimates.

With the completion of the three stages of our algorithm, we have all the information needed to compute the product

$$\prod_{m=1}^{M-1} (I + P_m) \tag{6·12}$$

which appears in (3·9) and which contributes the terms $p_{ij}$ to (3·14). Also, by (5·9), we have the information needed for the estimate (3·15) of $\eta_j$ which represents the error term in (3·14). Thus our algorithm computes the solutions (3·14) of (1·3) to a specified accuracy based on (3·15). We have of course chosen to orientate our discussion towards the example (6·1).

The computation associated with the product (6·12) can be implemented symbolically only for $M < 6$ since, for larger $M$, the number of terms that need to be manipulated becomes too large for the computer store that we have available, and the computation is performed numerically with an accuracy of 30 decimal digits. In

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Table 4. *Time in seonds for determining* (3·14) *with* $X = 10$, $\lambda = 1+i$

| | Symbolic calculation | | | Numeric calculation | | |
|---|---|---|---|---|---|---|
| $M$ | $\alpha = \frac{1}{2}$ | $\alpha = 1$ | $\alpha = \frac{4}{3}$ | $\alpha = \frac{1}{2}$ | $\alpha = 1$ | $\alpha = \frac{4}{3}$ |
| 4 | 120·65 | 17·5167 | 149·983 | 9·55 | 6·46667 | 13·8833 |
| 6 | — | 182·583 | — | 34·1333 | 11·2 | 40·5333 |
| 7 | — | 773·8 | — | 71·556 | 19·35 | 84·6667 |

Table 4 we give the times needed to compute (3·14) using symbolic and numerical methods. The shorter time needed when $\alpha = 1$ is a consequence of derivative terms, which are not zero for non-integer $\alpha$, becoming zero when $\alpha = 1$.

## 7. *Generalized Titchmarsh–Weyl theory*

The motivation for the asymptotic analysis and associated algorithm in Sections 2–6 is provided by the spectral theory of the equation

$$(-1)^{\nu} y^{(2\nu)} + q(x)\, y = \lambda y \quad (0 \leqslant x < \infty) \tag{7·1}$$

together with boundary conditions at $x = 0$. Here $q(x)$ is real-valued and locally integrable in $[0, \infty)$ and $\lambda$ is a complex spectral parameter. We take the boundary conditions to be the Dirichlet conditions

$$y^{(k-1)}(0) = 0 \quad (1 \leqslant k \leqslant \nu) \tag{7·2}$$

but we shall comment briefly on other choices of boundary conditions later in this section. Our purpose here is to state what we need from the spectral theory of (7·1), and then to introduce the contribution that our methods make.

The fundamental result of Titchmarsh and Weyl in [**25**, chapter 2] and [**27**] concerns the case $\nu = 1$ of (7·1) and (7·2), and they showed that, when $\operatorname{Im}\lambda \neq 0$, (7·1) has a non-trivial solution $\psi(x, \lambda)$ which is $L^2(0, \infty)$. The importance of this solution lies in writing $\psi$ in the form

$$\psi(x, \lambda) = \theta(x, \lambda) + m(\lambda)\, \phi(x, \lambda), \tag{7·3}$$

where $\theta$ and $\phi$ are the solutions of (7·1) (with $\nu = 1$) which satisfy the initial conditions

$$\theta(0, \lambda) = 1, \quad \theta'(0, \lambda) = 0; \quad \phi(0, \lambda) = 0, \quad \phi'(0, \lambda) = 1. \tag{7·4}$$

The function $m(\lambda)$ thus defined is the basis for the spectral theory of (7·1) and (7·2) as developed in [**25**, chapter 2] and [**27**] for the case $\nu = 1$. Depending on the nature of $q(x)$, either $m(\lambda)$ is uniquely determined for every non-real $\lambda$ (the so-called limit-point case) or $m(\lambda)$ involves an additional parameter (the limit-circle case). We refer to the paper by Fulton [**15**] for a more recent critical discussion of the limit-circle case. A number of explicit examples of $m(\lambda)$ are given in [**25**, chapter 4] for equations (7·1) which can be solved in terms of the special functions.

The generalization of the Titchmarsh–Weyl theory to higher-order equations, of which (7·1) is an instance, was made by Everitt [**13**], [**14**]. Here we indicate this generalization in the yet wider context of the Hamiltonian system

$$JY'(x) = \{\lambda A(x) + B(x)\}\, Y(x) \quad (0 \leqslant x < \infty), \tag{7·5}$$

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the spectral theory of which was initiated by Atkinson [**1**, chapter 9] and further developed by Hinton and Shaw in a series of papers which include [**17**], [**18**], [**19**]. In (7·5), $Y$ is a $2\nu$-component vector, $A$ and $B$ are Hermitian matrices with $A \geqslant 0$, and

$$J = \begin{pmatrix} 0 & -I_\nu \\ I_\nu & 0 \end{pmatrix}$$

in terms of the $\nu \times \nu$ identity matrix $I_\nu$. We note that (7·1) is the special case of (7·5) in which the entries $a_{ij}$ and $b_{ij}$ of $A$ and $B$ are

$$a_{11} = 1, \quad a_{ij} = 0 \text{ otherwise},$$
$$b_{11} = -q, \quad b_{2\nu,\,2\nu} = 1,$$
$$b_{ij} = 1 (j = i+\nu-1, 2 \leqslant i \leqslant \nu \text{ and } i = j+\nu-1, 2 \leqslant j \leqslant \nu),$$

and $b_{ij} = 0$ otherwise. The components $y_i$ of $Y$ are then given by

$$y_i = y^{(i-1)} (1 \leqslant i \leqslant \nu) = (-1)^i y^{(3\nu-i)} (\nu+1 \leqslant i \leqslant 2\nu). \tag{7·6}$$

We now introduce the Dirichlet boundary condition

$$(I_\nu 0)\, Y(0) = 0 \tag{7·7}$$

for (7·5), which corresponds to (7·2), and we also introduce the $2\nu \times \nu$ solution matrices $\Theta(x, \lambda)$ and $\Phi(x, \lambda)$ of (7·5) which satisfy the initial conditions

$$\Theta(0, \lambda) = \begin{pmatrix} I_\nu \\ 0 \end{pmatrix}, \quad \Phi(0, \lambda) = \begin{pmatrix} 0 \\ I_\nu \end{pmatrix}. \tag{7·8}$$

These conditions correspond to (7·4). In the references just cited, it is shown that, when $\operatorname{Im} \lambda \neq 0$, (7·5) has a $2\nu \times \nu$ solution matrix, with rank $\nu$, such that

$$\int_0^\infty \Psi^*(x, \lambda)\, A(x)\, \Psi(x, \lambda)\, dx < \infty. \tag{7·9}$$

Further, corresponding to (7·3), $\Psi$ can be written as

$$\Psi(x, \lambda) = \Theta(x, \lambda) + \Phi(x, \lambda)\, M(\lambda), \tag{7·10}$$

so defining the $\nu \times \nu$ matrix $M(\lambda)$. This matrix again forms the basis for the spectral theory of (7·5) and (7·7), as in the case of $m(\lambda)$ in (7·3).

By analogy with the Titchmarsh–Weyl theory, we say that (7·5) is in the limit-point case if, for some $\lambda$ with $\operatorname{Im} \lambda \neq 0$, (7·5) has no more than $\nu$ linearly independent solutions such that

$$\int_0^\infty Y^*(x, \lambda)\, A(x)\, Y(x, \lambda)\, dx < \infty.$$

This limit-point classification is independent of $\lambda$ and, by (7·9) and (7·10), it has the implication that $M(\lambda)$ is uniquely determined for all non-real $\lambda$. Further, if $\Psi_1(x, \lambda)$ is any other $2\nu \times \nu$ solution matrix of (7·5) which has rank $\nu$ and also satisfies (7·9), then

$$\Psi_1(x, \lambda) = \Psi(x, \lambda)\, C(\lambda) \tag{7·11}$$

for some non-singular $\nu \times \nu$ matrix $C$. It now follows from (7·8), (7·10) and (7·11) that

$$\Psi_1(0, \lambda) = \begin{pmatrix} C(\lambda) \\ M(\lambda)\, C(\lambda)) \end{pmatrix}.$$

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Hence, partitioning

$$\Psi_1(0,\lambda) = \begin{pmatrix} \zeta(\lambda) \\ \eta(\lambda) \end{pmatrix}, \tag{7·12}$$

we obtain

$$\zeta(\lambda) = C(\lambda), \quad \eta(\lambda) = M(\lambda)\, C(\lambda).$$

Eliminating $C(\lambda)$, we obtain a formulae for $M(\lambda)$ in terms of the initial values of $\Psi_1$ at $x = 0$:

$$M(\lambda) = \eta(\lambda)\, \zeta^{-1}(\lambda). \tag{7·13}$$

Finally here, we note that $M(\lambda)$ is analytic for $\operatorname{Im}\lambda \neq 0$ and $M(\lambda)$ coincides with its own transpose, that is, its entries satisfy $m_{ij}(\lambda) = m_{ji}(\lambda)$ [**18**].

For use in the next section, we mention here the form which (7·13) takes when (7·5) arises from the fourth-order example of (7·1) with $\nu = 2$. In this situation, we have two linearly indedpendent $L^2(0,\infty)$ solutions $\psi_1(x,\lambda)$ and $\psi_2(x,\lambda)$ of (7·1). Then, by (7·6), (7·12) and (7·13), the spectral matrix $M(\lambda) = (m_{ij}(\lambda))$ is given by

$$(m_{ij}(\lambda)) = \begin{pmatrix} -\psi_1'''(0,\lambda) & -\psi_2'''(0,\lambda) \\ \psi_1''(0,\lambda) & \psi_2''(0,\lambda) \end{pmatrix} \begin{pmatrix} \psi_1(0,\lambda) & \psi_2(0,\lambda) \\ \psi_1'(0,\lambda) & \psi_2'(0,\lambda) \end{pmatrix}^{-1}. \tag{7·14}$$

We have mentioned that examples of $m(\lambda)$ exist when $\nu = 1$ in (7·1), arising from the special functions. In contrast, no such examples are known when $\nu \geqslant 2$ except for the relatively trivial Fourier case when $q(x) = 0$. In order therefore to illustrate and test the general spectral theory of (7·1), there is a need for a computational approach to estimate $M(\lambda)$ numerically. Thus the motivation for our work is the development of an effective computational approach and, in the next section, we give our numerical results for the example where $\nu = 2$ and $q(x) = -x^\alpha$. Our methods are not confined to this choice of $q(x)$, but this choice does have a certain significance which we discuss in Section 10.

We have concentrated on the Dirichlet boundary conditions (7·2) and (7·7). If these are changed to other conditions which involve linear combinations of derivatives, then (7·8) and consequently $M(\lambda)$ are also changed. However, in the limit-point case emphasized here, the new $M(\lambda)$ is related to the Dirichlet $M_D(\lambda)$ by a functional equation, and therefore in principle the properties of the new $M(\lambda)$ can be obtained from those of $M_D(\lambda)$. We refer to [**25**, p. 69] and [**8** theorem 3·4] for the details of the functional equation. Here, as an example, we note only that, if (7·7) is replaced by the Neumann condition $(0 I_\nu)\, Y(0) = 0$, then [**8**, corollary 3·1]

$$M_N(\lambda) = -M_D^{-1}(\lambda).$$

## 8. *Computation of the spectral matrix*

We can now draw together the ideas in the previous sections to give an effective procedure for the numerical computation of the spectral matrix $(m_{ij}(\lambda))$ associated with the equation

$$y^{(4)} - x^\alpha y = \lambda y \quad (0 \leqslant x < \infty) \tag{8·1}$$

and the Dirichlet boundary conditions

$$y(0) = 0, \quad y'(0) = 0.$$

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The range for $\alpha$ is $0 < \alpha \leqslant 4/3$, so that (8·1) is in the limit-point case as required in section 7 [**11**, theorem 3·11·1(b)] and [**21**, section 23·4].

The $m_{ij}(\lambda)$ are given by (7·14) and we therefore require the values at $x = 0$ of two $L^2(0.\infty)$ solutions $\psi_1(x,\lambda)$ and $\psi_2(x,\lambda)$ of (8·1), together with the values of their derivatives. We take $\operatorname{Im}\lambda > 0$ to be definite. Then consideration of the exponential factor in (3·14), with $Q = \lambda + x^\alpha$ and $n = 4$, shows that the two $L^2(0,\infty)$ solutions of (8·1) are associated with $\omega_2$ and $\omega_3$. Thus (3·14) provides the values of $\psi_1(x,\lambda)$ and $\psi_2(x,\lambda)$ and their derivatives at $x = X$, with an error given by (3·15). These values are produced by our algorithm as explained at the end of Section 6, and we denote the maximum error in this computation by $\epsilon(X)$. The values of the solutions and their derivatives at $X$ are used as initial data for a numerical initial value solver which is then used to compute numerically the values of the solutions and their derivatives at 0. These values are then used in (7·14). This computation back to $x = 0$ has been performed with the NAG library code D02NMF in the following way. We introduce the standard Riccati variable $\xi(x) = \sigma(x)\,\tau^{-1}(x)$, where

$$\sigma = \begin{pmatrix} \psi_1 & \psi_2 \\ \psi_1' & \psi_2' \end{pmatrix}, \quad \tau = \begin{pmatrix} -\psi_1''' & -\psi_2''' \\ \psi_1'' & \psi_2'' \end{pmatrix}.$$

Then, as in [**2**], $\xi$ satisfies a first-order nonlinear differential equation. The above code is applied to $\xi$, and it computes $\xi$ back from $X$ to 0. Then, by (7·14), $M(\lambda) = \xi^{-1}(0)$.

The value of $X$ is at our disposal, and the actual choice is governed by two factors. A smaller choice has the advantage that the integration back from $X$ to zero is performed over a smaller range with a better retention of the accuracy represented by $\epsilon(X)$. On the other hand, a larger choice has the advantage that $\epsilon(X)$ is smaller. The first factor appears to be more significant and we have chosen $X = 10$. Later we shall comment on $X = 20$ and on the very large values of $X$ that arise in the alternative method of Bennewitz *et al.*[**2**]. The value of $M$ – the number of requested transformations in Sections 3–6 – is also at our disposal, and we have chosen $M = 6$ to obtain the good accuracy which we present later in Tables 5–7. We turn now to discuss the results of numerical experiments performed with our algorithm. In Tables 5–7 we give the values of $m_{11}(\lambda)$, $m_{22}(\lambda)$ and $m_{12}(\lambda) = m_{21}(\lambda)$ for three values of $\alpha$ and a selection of values of $\lambda$. The values of $\alpha$ are, first, $\alpha = 1$ because in this case we can obtain independent confirmation of our results from the theory of the higher-order Airy equation, which is the subject of Section 9. Then $\alpha = 4/3$ is chosen because it is the maximum value of $\alpha$ for which (8·1) remains in the limit-point case. Finally $\alpha = 1/2$ is chosen in order to give a spread of values of $\alpha$ in the range $0 < \alpha \leqslant 4/3$.

The values of $\lambda$, all with $\operatorname{Im}\lambda > 0$, are mainly taken to be near the origin because we wish to compare the power of our method with that of the code developed previously by Bennewitz *et al.*[**2**]. Our method is considerably more effective, and the improvement is most conspicuous for smaller values of $|\lambda|$, particularly when $\alpha = 4/3$, as can be seen from Table 6 and the choice of $X$ in the other tables. We recall that a value of $X$ as small as possible is generally the most desirable because of the integration of (8·1) over $[0, X]$ starting from initial values at $X$.

8·1 *Example* $\alpha = 1$. We have carried out the computation using $M = 6$ in the algorithm in Section 6. With $X = 10$ and $X = 20$, we obtain

$$\epsilon(10) = 2{\cdot}036\,696 \times 10^{-6}, \quad \epsilon(20) = 1{\cdot}038\,152 \times 10^{-8}.$$

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Table 5. $\alpha = 1$

| $\lambda$ | Asymptotic solution: Numerical integration: Over $[0,10]$ | Asymptotic solution: Numerical integration: Over $[0,20]$ | Bennewitz: Accuracy | Bennewitz: Integration distance $X$ |
|---|---|---|---|---|
| i | $-0{\cdot}184432148\,9+1{\cdot}822040557\,9$ i | 10 sf | 10 sf | 11755·07 |
| | $-0{\cdot}661380112\,2+1{\cdot}103073597\,0$ i | 10 sf | 10 sf | — |
| | $-1{\cdot}429114222\,5+0{\cdot}840139269\,8$ i | 10 sf | 10 sf | — |
| 0·5 + i | $0{\cdot}193507388\,2+2{\cdot}056052684\,8$ i | 8 sf | Failed | 74606·02 |
| | $-0{\cdot}587145268\,9+1{\cdot}256146192\,6$ i | 8 sf | — | — |
| | $-1{\cdot}440704226\,5+0{\cdot}932785391\,8$ i | 8 sf | — | — |
| 10 + 10 i | $2{\cdot}086848020\,6+10{\cdot}297162056\,0$ i | 10 | 10 sf | 59·15 |
| | $-1{\cdot}453293919\,6+3{\cdot}544100046\,2$ i | 10 | 10 sf | — |
| | $-2{\cdot}304608106\,6+1{\cdot}547645330\,4$ i | 10 | 10 sf | — |
| 1 + 0·001 i | $1{\cdot}072600603\,1+1{\cdot}605358243\,0$ i | 7 sf | — | Failed |
| | $-0{\cdot}216280162\,3+1{\cdot}315539836\,9$ i | 7 sf | — | — |
| | $-1{\cdot}296726703\,6+1{\cdot}078308701\,5$ i | 7 sf | — | — |
| 0·01 i | $0{\cdot}327181488\,3+1{\cdot}033072352\,4$ i | 7 sf | — | Failed |
| | $-0{\cdot}214900970\,5+0{\cdot}880202412\,6$ i | 10 sf | — | — |
| | $-0{\cdot}312744021\,4+0{\cdot}951555907\,7$ i | 7 sf | — | — |

Table 6. $\alpha = \frac{4}{3}$

| $\lambda$ | Asymptotic solution | Bennewitz: Accuracy | Bennewitz: Integration distance $X$ |
|---|---|---|---|
| i | $-0{\cdot}279032558\,2+1{\cdot}832344770\,4$ i | — | Failed |
| | $-0{\cdot}715393602\,8+1{\cdot}102572917\,9$ i | — | — |
| | $-1{\cdot}471243500\,7+0{\cdot}829346597\,2$ i | — | — |
| 0·5 + i | $0{\cdot}097469888\,6+2{\cdot}055709362\,0$ i | — | Failed |
| | $-0{\cdot}638426125\,0+1{\cdot}246791720\,4$ i | — | — |
| | $-1{\cdot}476808309\,6+0{\cdot}915723860\,3$ i | — | — |
| 10 + 10 i | $2{\cdot}043056488\,0+10{\cdot}271134376\,5$ i | 6 sf | 290·36 |
| | $-1{\cdot}462924361\,2+3{\cdot}531812667\,8$ i | 6 sf | — |
| | $-2{\cdot}307085752\,5+1{\cdot}541545748\,7$ i | 6 sf | — |
| 1 + 0·001 i | $0{\cdot}958453416\,8+1{\cdot}586784243\,6$ i | — | Failed |
| | $-0{\cdot}274101883\,2+1{\cdot}285582184\,8$ i | — | — |
| | $-1{\cdot}329403877\,3+1{\cdot}041808366\,8$ i | — | — |
| 0·01 i | $0{\cdot}201005876\,1+1{\cdot}045929908\,8$ i | — | Failed |
| | $-1{\cdot}273800730\,7+0{\cdot}849220812\,3$ i | — | — |
| | $-0{\cdot}392628580\,3+0{\cdot}940552294\,3$ i | — | — |

The numerical integration over $[0, X]$ is performed with an accuracy of $10^{-10}$. Eight values of $\lambda$ are considered, as listed in Table 5. In the third column, the agreement in terms of significant figures is given for the choice $X = 20$. The slight loss of accuracy is in line with the comments which we made earlier in this section concerning the choice of $X$. The last two columns give the corresponding performance of the code of Bennewitz *et al.*[**2**]. The large values of $X$ and the cases of failure will be noted, as will also the cases of agreement.

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Table 7. $\alpha = \frac{1}{2}$

| $\lambda$ | Asymptotic solution | Bennewitz | |
|---|---|---|---|
| | | Accuracy | Integration distance $X$ |
| i | 0·091 168 865 2 + 1·807 941 198 3 i | 7 sf | 174·35 |
| | −0·569 654 822 3 + 1·101 846 098 9 i | 7 sf | — |
| | −1·359 921 693 8 + 0·852 317 631 2 i | 10 sf | — |
| 0·5 + i | 0·389 911 204 6 + 2·059 663 534 2 i | 6 sf | 193·55 |
| | −0·499 729 365 1 + 1·270 027 756 7 i | 7 sf | — |
| | −1·382 011 771 2 + 0·956 399 679 2 i | 7 sf | — |
| 10 + 10 i | 2·200 807 094 6 + 10·347 609 520 0 i | 6 sf | 33·84 |
| | −1·430 869 698 5 + 3·566 433 668 1 i | 6 sf | — |
| | −2·299 158 811 6 + 1·557 829 380 0 i | 7 sf | — |
| 1 + 0·001 i | 1·297 133 088 1 + 1·638 462 781 9 i | — | Failed |
| | −0·119 985 170 7 + 1·362 653 017 0 i | — | — |
| | −1·245 826 005 9 + 1·133 554 101 0 i | — | — |
| 0·01 i | 0·575 828 135 0 + 1·016 704 917 0 i | — | 243 897·42 |
| | −1·116 694 808 0 + 0·933 435 082 4 i | — | — |
| | −0·175 737 857 8 + 0·971 949 756 1 i | — | — |

8·2. *Example* $\alpha = 4/3$. We have again carried out the computations using $M = 6$, and we obtain

$$\epsilon(10) = 6{\cdot}57898 \times 10^{-6}.$$

Table 6 gives the values of $m_{ij}$ for eight values of $\lambda$ as before and the choice $X = 10$. In the last two columns of the table, the poor performance of the previous code [**2**] will be noted.

8·3. *Example* $\alpha = 1/2$. Again with $M = 6$, we obtain

$$\epsilon(10) = 1{\cdot}452\,392 \times 10^{-6}$$

and the values of the $m_{ij}$ are given in Table 7. This time the previous code [**2**] performs better but it still does not match ours. It will be noted, in all three numerical examples that we discuss, that our methods produce results that are in agreement with the results in [**2**]. Further the algorithm reported on in [**2**] fails to compute the spectral matrix for values of $\lambda$ close to the real line. Our algorithm has no difficulty computing the spectral matrix at these values.

## 9. *The higher-order Airy equation*

Independent confirmation of our numerical results for the case $\alpha = 1$ in Example 8·1 is provided by the theory of the equation

$$\frac{d^n y}{dz^n} = (-1)^n zy \tag{9·1}$$

which, when $n = 2$, becomes the well-known Airy equation. We note that (9·1) is itself a special case of the equation

$$\frac{d^n y}{dz^n} = (-1)^n z^m y,$$

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with $m$ rational, which has been extensively investigated by Turrittin[**26**], Heading[**16**], and others (see also Paris and Wood[**22**, pp. 188–190]). Here $z$ is a complex variable and, when

$$z = \lambda + x \tag{9·2}$$

and $n = 4$, (9·1) becomes

$$y^{(4)}(x) = (\lambda + x)\, y(x), \tag{9·3}$$

which is the case $\alpha = 1$ of (8·1). Thus we consider the equation

$$\frac{d^4y}{dz^4} = zy \tag{9·4}$$

and our primary source for the nature of the solutions is the paper by Heading[**16**, sections 1–5].

We note first that a straightforward power series substitution for $y$ in (9·4) gives the general solution in the form

$$y(z) = \sum_{r=0}^{3} c_r z^r f_r(z), \tag{9·5}$$

where the $c_r$ are constants and

$$\begin{aligned}
f_0(z) &= 1 + \frac{1!}{5!}z^5 + \frac{1!6!}{5!10!}z^{10} + \frac{1!6!11!}{5!10!15!}z^{15} + \dots,\\
f_1(z) &= 1 + \frac{2!}{6!}z^5 + \frac{2!7!}{6!11!}z^{10} + \frac{2!7!12!}{6!11!16!}z^{15} + \dots,\\
f_2(z) &= 1 + \frac{3!}{7!}z^5 + \frac{3!8!}{7!12!}z^{10} + \frac{3!8!13!}{7!12!17!}z^{15} + \dots,\\
f_3(z) &= 1 + \frac{4!}{8!}z^5 + \frac{4!9!}{8!13!}z^{10} + \frac{4!9!14!}{8!13!18!}z^{15} + \dots,
\end{aligned} \tag{9·6}$$

and the power series converge for all $z$. As mentioned by Heading[**16**, p. 405], the $f_r$ can if necessary be expressed in terms of the generalized hypergeometric function ${}_0F_3$: for example

$$f_0(z) = {}_0F_3(4/5, 3/5, 2/5; z^5/5^4).$$

A particular choice of the constants $c_r$ is identified by Heading as producing solutions which have specific asymptotic behaviours for large $|z|$. The choice [**16**, (37)] is

$$\begin{aligned}
c_0 &= \Gamma(\tfrac{1}{5})\,\Gamma(\tfrac{2}{5})\,\Gamma(\tfrac{3}{5}),\\
c_1 &= \Gamma(-\tfrac{1}{5})\,\Gamma(\tfrac{1}{5})\,\Gamma(\tfrac{2}{5})\,5^{-4/5},\\
c_2 &= \Gamma(-\tfrac{2}{5})\,\Gamma(-\tfrac{1}{5})\,\Gamma(\tfrac{1}{5})\,5^{-8/5},\\
c_3 &= \Gamma(-\tfrac{3}{5})\,\Gamma(-\tfrac{2}{5})\,.\,\Gamma(-\tfrac{1}{5})\,5^{-12/5}.
\end{aligned} \tag{9·7}$$

Then, as in [**16**, (24), (37), (38)], we denote the solution (9·5) with this choice by $J(z)$. It is shown in [**16**, (39)] that

$$J(z) \sim (\text{const.})\, z^{-3/8} \exp(-\tfrac{4}{5}z^{5/4}) \tag{9·8}$$

for large $|z|$ with $\arg z \neq \pi$, and we can use this asymptotic formula to find the two $L^2(0, \infty)$ solutions $\psi_1(x, \lambda)$ and $\psi_2(x, \lambda)$ of (9·3) when $\operatorname{Im}\lambda \neq 0$.

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First, with $z = x+\lambda$ as in (9·2), it is clear from (9·8) that $J(x+\lambda)$ is exponentially small as $x \to \infty$ and hence is $L^2(0, \infty)$. Thus

$$\psi_1(x, \lambda) = J(x+\lambda) = \sum_{r=0}^{3} c_r (x+\lambda)^r f_r(x+\lambda), \tag{9·9}$$

where the $f_r$ and $c_r$ are defined by (9·6) and (9·7).

Secondly, as observed in [**16**, (25)], $y(\omega z)$ is also a solution of (9·4) whenever $y(z)$ is a solution and $\omega^5 = 1$. We therefore consider

$$\psi_2(x, \lambda) = J\{(x+\lambda)\,\epsilon^{-2\pi i/5}\} = \sum_{r=0}^{3} c_r\, e^{-2\pi i r/5} (x+\lambda)^r f_r(x+\lambda). \tag{9·10}$$

For this solution, the exponential factor in (9·8) is

$$\exp\{\tfrac{4}{5}i(x+\lambda)^{\frac{5}{4}}\} = \exp\{\tfrac{4}{5}ix^{\frac{5}{4}}(1+\tfrac{5}{4}\lambda x^{-1}+O(x^{-2}))\},$$

and the modulus of this factor is

$$\{1+O(x^{-\frac{3}{4}})\}\exp\{-\operatorname{Im}\lambda)\, x^{\frac{1}{4}}\}.$$

Hence, when $\operatorname{Im}\lambda > 0$, $\psi_2(x, \lambda)$ is also exponentially small as $x \to \infty$ and is therefore $L^2(0, \infty)$.

The initial values of $\psi_1$ and $\psi_2$ at $x = 0$ are now known in terms of $\lambda$ from (9·9) and (9·10), and therefore (7·14) provides an explicit formula for $M(\lambda)$ in terms of power series involving $\lambda$. In using this formula to verify our computations in Example 8·1, we have approximated $\psi_1(x, \lambda)$ and $\psi_2(x, \lambda)$ by using the first 20 terms of the power series given in (9·5) and (9·6). Expressions for the derivatives have been calculated symbolically, and the evaluation of $\psi_1(0, \lambda), \psi_2(0, \lambda)$ and the derivatives has been performed with 30 digits of accuracy.

## 10. *Concluding remarks*

(*a*) *The algorithm of Bennewitz et al.*[**2**]. We have already referred to some numerical results of the algorithm [**2**] in Section 8 when $q(x) = -x^\alpha$. A more general comment on the algorithm is that it works well in cases where $M(\lambda)$ is meromorphic, as for example when $q(x) = x^\alpha (\alpha > 0)$. However, the computational complexity of the method causes the performance to degrade and even fail for examples of (7·1) when $\arg\lambda$ is small and $M(\lambda)$ is not meromorphic. It is partly for this reason that we have concentrated on $q(x) = -x^\alpha$, $(0 < \alpha \leqslant 4/3)$, the spectrum in this case filling the whole real axis [**21**, section 24·4] with, consequently, $M(\lambda)$ being non-meromorphic. This is the wider context within which to place our comments in Section 8 concerning the effectiveness of our methods as compared to those of [**2**].

(*b*) HELP *inequalities*. In the case $\nu = 1$ of (7·1), the behaviour of $m(\lambda)$ in the neighbourhood of $\lambda = 0$ determines the validity of what is known as the HELP (Hardy–Everitt–Littlewood–Polya) inequality. We refer to [**4**] and [**12**] for surveys and an extensive bibliography concerning the inequality. An extension to fourth-order differential equations was given by Russell[**23**][**24**], but recently a more systematic development for (7·1) with general $\nu$ has been given by Dias[**8**]. Again the validity of an inequality of the HELP type depends on the behaviour of $M(\lambda)$ near to $\lambda = 0$. Having in this paper developed a computational algorithm which is

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effective for small $|\lambda|$, we propose to investigate further the application to the validity of higher-order HELP inequalities.

(*c*) *Coefficients with an oscillatory factor*. It is pointed out in [**11**, example 2·4·1] that the method of repeated diagonalization for (1·2) works not only for coefficients of the type (5·1) but also for coefficients such as

$$Q(x) = x^{\alpha} p(x^{\beta})$$

with $\beta > 0$ and $p(t)$ periodic in $t$ and nowhere zero. It seems likely that, with suitable modifications to the algorithm in Section 6, the methods of this paper will cover such a coefficient in (1·3). It would appear that a higher value of $M$ than (5·15) is needed to achieve the same accuracy (5·8) as before and that the grouping of terms in the algorithm of Sections 5 and 6 depends on the value of $\beta$. These details are another matter for further investigation.

(*d*) *Hamiltonian systems in general*. We have concentrated in this paper on the equations (1·3) and, for the spectral theory, (7·1). However, our methods are in principle applicable to other differential equations and indeed Hamiltonian systems which, after an initial transformation, can be written in the form (3·1) with $\Lambda$ similar to (3·2). Such a $\Lambda$ would be

$$\Lambda = \rho(x)\,\mathrm{dg}\,(d_1, \ldots, d_n),$$

where there is a factor $\rho(x)$ and the $d_k$ are distinct non-zero constants. More difficult however – and this is the point of this subsection – are systems (3·1) where the diagonal terms in $\Lambda$ have different orders of magnitude as $x \to \infty$. Such a situation can occur for example with the equation

$$y^{(4)}(x) + \{P(x)\,y'(x)\}' + Q(x)\,y(x) = 0,$$

where the middle coefficient is dominant in the sense that $Q = o(P^2)$ as $x \to \infty$ [**11**, section 3·5]. Thus a further stage in the development of our asymptotic analysis and the associated algorithm would be to cope with differential equations, and more generally Hamiltonian systems, where this type of $\Lambda$ occurs.

(*e*) *Automatic differentiation*. The algorithm discussed in this paper has been developed using both *Mathematica and Fortran77*. This has resulted in some computationally intensive symbolic calculations as is demonstrated by the results in Tables 2 and 3. A possible alternative approach to performing the computation would be to use an automatic differentiation package to evaluate numerically the required derivatives. Such an approach would mean that the complete algorithm could be implemented in, say, *Fortran 77* or *Fortran 90*, thus avoiding both the long symbolic calculations reported on in Section 6, and also the need to interface the Fortran code to the *Mathematica* package. We intend to address this issue in a future publication.

(*f*) *Provably correct computations*. There is a considerable interest in performing provably correct computations. We note that the symbolic algorithm described in Section 6 provides, not only an estimate of the $L^2[0, \infty)$ solution at some point $X > 0$, but also a provably correct bound on the error at $X$. This information could be used as input data to an interval-based ordinary differential equation solver, and the computation of the $M(\lambda)$ spectral matrix could be performed in a provably correct manner, giving precise information on the numerical errors involved. The effectiveness of this approach will need further investigation.

https://doi.org/10.1017/S0305004196001491 Published online by Cambridge University Press

*Acknowledgement*. The authors wish to thank the EPSRC for grant GR/J61442 under which this research has been supported.

REFERENCES

[1] F. V. Atkinson. *Discrete and continuous boundary value problems* (Academic Press, 1964).
[2] C. Bennewitz, B. M. Brown, W. D. Evans, D. K. R. McCormack and M. Marletta. Computation of the $m$ matrix for fourth order problems, *Proc. Roy. Soc. Lond*, A, **452** (1996), 1765–1788.
[3] B. M. Brown, M. S. P. Eastham, W. D. Evans and V. G. Kirby. Repeated diagonalization and the numerical computation of the Titchmarsh–Weyl $m(\lambda)$ function. *Proc. Roy. Soc. Lond*. A, **445** (1994), 113–126.
[4] B. M. Brown, W. D. Evans and W. N. Everitt. HELP integral and series inequalities; in *Proceedings of the VI meeting on General Inequalities, Oberwolfach 1990* (Ed. W. Walter) International Series of Numerical Mathematics, vol. 103, 1990, 269–305.
[5] J. S. Cassell. An extension of the Liouville–Green asymptotic formula for oscillatory formula for oscillatory second-order differential equations. *Proc. Roy. Soc. Edin.*, **100** (1985), 181–190.
[6] J. S. Cassell. Generalised Liouville–Green asymptotic approximations for second-order differential equations. *Proc. Roy. Soc. Edin.*, **103** A (1986), 229–239.
[7] J. S. Cassell. Liouville–Green asymptotic theory for second-order equations with complex coefficients. *Quart. J. Math.* (*Oxford*), (2) **39** (1988), 135–149.
[8] N. G. J. Dias. On an integral inequality associated with a $2n$th order quasi-differential expression (PhD thesis, Cardiff; University of Wales, 1994).
[9] M. S. P. Eastham. A repeated transformation in the asymptotic solution of linear differential systems. *Proc. Roy. Soc. Edin.*, **102** A (1986), 173–188.
[10] M. S. P. Eastham. Repeated diagonalization and extended Liouville–Green asymptotic formulae. *J. London Math. Soc.* (2) **36** (1987), 115–125.
[11] M. S. P. Eastham. *The asymptotic solution of linear differential systems* (Clarendon Press, 1989).
[12] W. D. Evans and W. N. Everitt. A return to the Hardy–Littlewood inequality. *Proc. Roy. Soc. Lond.* A **380** (1982), 447–486.
[13] W. N. Everitt. Fourth-order singular differential equations. *Math. Ann.* **149** (1963), 320–340.
[14] W. N. Everitt. Singular differential equations I: the even order case. *Math. Ann.* **156** (1964), 9–24.
[15] C. T. Fulton. Parameterization of Titchmarsh's $m(\lambda)$-functions $m(\lambda)$-functions in the limit-circle case. *Trans. Amer. Math. Soc.* **229** (1977), 51–63.
[16] J. Heading. The Stokes phenomenon and certain $n$th-order differential equations. I. *Proc. Camb. Phil. Soc.* **53** (1957), 399–418.
[17] D. B. Hinton and J. K. Shaw. Titchmarsh–Weyl theory for Hamiltonian systems; in *Spectral theory of differential operators*. I. (Eds. W. Knowles and R. T. Lewis) pp. 219–231 (North-Holland, 1981).
[18] D. B. Hinton and J. K. Shaw. On Titchmarsh–Weyl $m(\lambda)$-functions for Hamiltonian systems. *J. Diff. Equations* **40** (1981), 316–342.
[19] D. B. Hinton and J. K. Shaw. On the spectrum of a singular Hamiltonian system. *Quaestiones Mathematicae* **5** (1982), 29–81.
[20] N. Levinson. The asymptotic nature of solutions of linear systems of differential equations. *Duke Math. J.* **15** (1948), 111–126.
[21] M. A. Naimark. *Linear differential operators. Part 2* (Harrap, 1968).
[22] R. B. Paris and A. D. Wood. *Asymptotics of high order differential equations*. Pitman Research Notes in Mathematics **129** (Longman, 1986).
[23] A. Russell. On a fourth-order singular integral inequality. *Proc. Roy. Soc. Edin.* A **80** (1978), 249–260.
[24] A. Russell. On certain fourth-order integral inequalities. *Proc. Roy. Soc. Edin.* A **83** (1979), 205–211.
[25] E. C. Titchmarsh. *Eigenfunction expansions, Part 1* (2nd ed.) (Clarendon Press, 1962).
[26] H. L. Turrittin. Stokes multipliers for asymptotic solutions of a certain differential equation. *Trans. Amer. Math. Soc.* **68** (1950), 304–329.
[27] H. Weyl. Über gewöhnliche Differentialgleichungen mit Singularitäten und die zugehörigen Entwicklungen willkürlicher Funktionen. *Math. Ann.* **68** (1910), 220–269.

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