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Spectral concentration and perturbed discrete spectra

B.M. Brown *, M.S.P. Eastham, D.K.R. McCormack

Department of Computer Science, University of Cardiff, Cardiff, CF2 3XF, UK

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Abstract

We examine spectral concentration for a class of Sturm–Liouville problems on $[0,\infty)$, a typical example being $y''(x)+(\lambda-x+cx^2)y(x)=0$. The discrete spectrum for $c=0$ leads to spectral concentration in the continuous spectrum for $c>0$, and we use a new formula for the spectral function to make a detailed computational investigation of the way in which spectral concentration occurs. In particular, we find that, as c decreases, spectral concentration arises first from the lowest unperturbed eigenvalue and then in turn from these eigenvalues in increasing order of size.

Keywords: Special concentration; Sturm–Liouville problems; Prüfer transformation

AMS classification: 34A12

1. Introduction

We consider the spectral function $\rho(\mu)$ $(-\infty<\mu<\infty)$ which is associated with the Sturm–Liouville equation

$$y''(x)+\{\lambda-q(x)\}y(x)=0 \quad (0\leqslant x<\infty) \tag{1.1}$$

and the boundary condition

$$y(0)=0. \tag{1.2}$$

Here, as usual, λ is a complex spectral parameter and q is real-valued and locally integrable in $[0,\infty)$. Also, the Dirichlet condition (1.2) is selected only for convenience: we can equally take the Neumann condition $y'(0)=0$ or generally $a_1y(0)+a_2y'(0)=0$ with real a_1 and a_2. The standard definition of $\rho(\mu)$ in terms of the Titchmarsh–Weyl function $m(\lambda)$ is

$$\rho(\mu)=\pi^{-1}\lim\int_0^{\mu}\operatorname{Im} m(t+\mathrm{i}\varepsilon)\,\mathrm{d}t \quad (\varepsilon\to 0), \tag{1.3}$$

* Corresponding author. E-mail: malcolm.brown@cs.cf.ac.uk

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and $m(\lambda)$ is uniquely defined when (1.1) is in the limit-point case. We refer to the standard works [4, Ch. 9; 5, Ch. 2; 19, Chs. 2–3] for the definition (1.3) and for the central role of ρ in the expansion theory of (1.1) and (1.2). It is known that ρ is nondecreasing and, following [3, 10], we say that spectral concentration occurs at a point μ_0 if

(a) ρ' exists and is continuous in a neighbourhood of μ_0 and

(b) ρ' has a local maximum at μ_0.

In a recent paper [3], we considered the case where q is $L(0,\infty)$, ρ then being absolutely continuous in $[0,\infty)$, and we developed computational procedures to locate spectral concentration for certain types of potential q, typical of which is $q(x) = -ce^{-ax}\cos x$ $(a>0,\ c>0)$. These procedures were based on a new theoretical formula

$$\rho'(\mu) = \pi^{-1}\mu^{1/2}\exp\left(-\mu^{-1/2}\int_0^\infty q(x)\sin 2\theta(x,\mu)\,\mathrm{d}x\right) \tag{1.4}$$

in which $\mu>0$ and θ is the solution of the first-order differential equation

$$\theta'(x,\mu) = \mu^{1/2} - \mu^{-1/2}q(x)\sin^2\theta(x,\mu) \tag{1.5}$$

such that $\theta(0,\mu)=0$. As pointed out in [3], the origin of (1.4) lies in the early work of Titchmarsh [18, Section 5.8] and Weyl [20, p. 264].

In this paper, we develop the ideas in [3] to apply also to situations where $q(x)\to-\infty$ as $x\to\infty$. In such a situation, it is known that ρ is absolutely continuous in the whole of $(-\infty,\infty)$ if q satisfies the conditions

$$\int_0^\infty q'|q|^{-5/2}<\infty, \qquad \int_0^\infty |q''||q|^{-3/2}<\infty, \qquad \int_0^\infty |q|^{-1/2}=\infty. \tag{1.6}$$

Proofs of the absolute continuity of ρ involve either an explicit representation of ρ' [19, Section 5.10, 20, p. 264] or the general concept of subordinacy [6, 15]. In this paper, we show that there is a formula for ρ' corresponding to (1.4) which can again be used as a basis for a computational investigation of ρ. This formula is given in Section 2. Then in subsequent sections we focus our application of the formula on the two examples:

$$\text{(i)}\quad q(x) = -cx^2 + x, \tag{1.7}$$

$$\text{(ii)}\quad q(x) = -cx - (1+x)^{-1}, \tag{1.8}$$

where c (>0) is considered as a small parameter.

There is a considerable literature on potentials typified by (1.7) and (1.8) based on the observation that, while the spectrum is continuous in $(-\infty,\infty)$ for all c (>0) however small, the unperturbed spectrum for $c=0$ is discrete in $(-\infty,\infty)$ and $(-\infty,0)$, respectively. The question then is to determine the influence of the discrete spectrum on the perturbed spectral problem with $c>0$. We refer to [7–9, 13] for extensive surveys of the literature which goes back to the papers of Schrödinger [14] and Oppenheimer [12]. A feature of this literature is the identification of non-real spectral points, known as resonances, which approximate to the unperturbed eigenvalues as $c\to0$ and, in terms of c, have exponentially small imaginary parts [1, 7, 8, Ch. 22]. In particular, we mention the perturbation theory of Titchmarsh [16–18, Ch. 20], see also [11], in which the Green's function for $\operatorname{Im}\lambda>0$ is analytically continued into the lower half-plane $\operatorname{Im}\lambda<0$, and the nonreal spectral points arise as poles of the continued function. In the case of (1.7), Titchmarsh obtained the real approximation

$$\lambda_n - \tfrac{8}{15}c\lambda_n^2 \tag{1.9}$$

to the nonreal spectral points, λ_n being an unperturbed eigenvalue [18, Section 19.18].

Our contribution in this paper is to use the new formula for ρ' to exhibit for the first time the influence of the unperturbed discrete spectrum on ρ itself. As c decreases, our computational results show that spectral concentration appears first near to the lowest unperturbed eigenvalue λ_0 and then additionally near the higher eigenvalues in turn. Our methods are entirely real-variable, and it is an open question whether there is a theoretical connection between the size of the imaginary parts of the resonances and the sharpness of the maxima of ρ' which we exhibit in this paper.

2. An expression for the spectral function

In this section, we consider (1.1) with $\lambda=\mu$ (real), and the basic conditions on q are (1.6). To accommodate (1.7), we suppose that q has the form

$$q(x) = -cs(s) + p(x), \tag{2.1}$$

where $c>0$, s and p are non-negative on $[0,\infty)$, $p(x)\to\infty$ and $p(x)=o\{s(x)\}$ as $x\to\infty$. The unperturbed spectrum consists of discrete positive eigenvalues, and therefore our interest is in $\mu>0$. We deal with (1.8) later, in Section 6. We make the Liouville–Green transformation

$$\xi = \int_0^x \{\mu + cs(t)\}^{1/2}\,\mathrm{d}t, \qquad \eta = \{\mu + cs(x)\}^{1/4} y \tag{2.2}$$

to express (1.1) as

$$\frac{\mathrm{d}^2\eta}{\mathrm{d}\xi^2} + \{1 + R(\xi,\mu)\}\eta = 0, \tag{2.3}$$

where

$$R(\xi,\mu) = -\frac{1}{4}c\frac{s''(x)}{\{\mu+cs(x)\}^2} + \frac{5}{16}c^2\frac{s'^2(x)}{\{\mu+cs(x)\}^3} - \frac{p(x)}{\mu+cs(x)} \tag{2.4}$$

and $x=x(\xi)$ by (2.2).

To obtain the formula for ρ' which corresponds to (1.4), we use the theory of Titchmarsh [19, Section 5.10]. Thus, in Titchmarsh's notation for $a(\mu)$ and $b(\mu)$,

$$\begin{aligned}\rho'(\mu) &= \pi^{-1}\{a^2(\mu)+b^2(\mu)\}^{-1}\\ &= \pi^{-1}\lim_{x\to\infty}[\{-q(x)\}^{1/2}\phi^2(x,\mu) + \{-q(x)\}^{-1/2}\phi'^2(x,\mu)],\end{aligned}$$

where ϕ is the solution of (1.1) (with $\mu=\lambda$) such that

$$\phi(0,\mu)=0, \qquad \phi'(0,\mu)=1. \tag{2.5}$$

The transformation (2.2), with $y = \phi$, gives

$$\rho'(\mu) = \pi^{-1} \lim\{\eta^2(\xi) + \eta'^2(\xi)\}^{-1}, \quad (\xi \to \infty) \tag{2.6}$$

where the prime attached to η denotes ξ-differentiation. We note that the initial conditions for η corresponding to (2.5) are

$$\eta(0) = 0, \quad \eta'(0) = \{\mu + \mathrm{cs}(0)\}^{-1/4}. \tag{2.7}$$

Now (2.6) can be represented in a convenient form by means of the Prüfer transformation

$$\eta(\xi) = r(\xi)\sin\theta(\xi), \qquad \eta'(\xi) = r(\xi)\cos\theta(\xi). \tag{2.8}$$

Then

$$r^2(\xi) = \eta^2(\xi) + \eta'^2(\xi) \tag{2.9}$$

and (2.3) is equivalent to the usual first-order equations

$$\theta'(\xi) = 1 + R(\xi,\mu)\sin^2\theta(\xi), \tag{2.10}$$

$$r'(\xi)/r(\xi) = -\tfrac{1}{2}R(\xi,\mu)\sin 2\theta(\xi). \tag{2.11}$$

Of course, r and θ also depend on μ as well as ξ. We note that (2.7) and (2.9) give $r(0) = \{\mu + cs(0)\}^{-1/4}$, while (2.7) and (2.8) give

$$\theta(0) = 0. \tag{2.12}$$

It now follows from (2.6) and integration of (2.11) that

$$\rho'(\mu) = \pi^{-1}\{\mu + cs(0)\}^{1/2} \exp\left(\int_0^\infty R(\xi,\mu)\sin 2\theta(\xi)\,\mathrm{d}\xi\right). \tag{2.13}$$

The convergence of the infinite integral here is naturally a consequence of the existence of the finite limit in (2.6). Thus our procedure for computing $\rho'(\mu)$ is first to compute $\theta(\xi)$ as the solution of (2.10) satisfying the initial condition (2.12), and then to use the result to evaluate the integral in (2.13). We give the procedure in more detail in Section 4 but first we describe the nature of θ in relation to spectral concentration.

3. The function θ

In [3] it was shown that the occurrence of spectral concentration is reflected in a rapid transitional behaviour of the function $\theta(x,\mu)$ which appears in (1.4) and (1.5). This behaviour arises as μ increases through a point μ_0 of spectral concentration and, in [3, Section 2], it relates to an interval (x_1,x_2) in which the Sturm–Liouville coefficient $\mu - q(x) < 0$. The function θ in (2.10) and (2.13) also exhibits similar behaviour which we introduce now in purely descriptive terms. We indicate the dependence of θ on μ by writing $\theta(\xi,\mu)$.

Let (ξ_1,ξ_2) be an interval in which the coefficient $1 + R$ in (2.3) is negative, and let μ' and μ'' be suitably close to a point μ_0 of spectral concentration with $\mu' < \mu_0 < \mu''$. Of course, ξ_1 and ξ_2

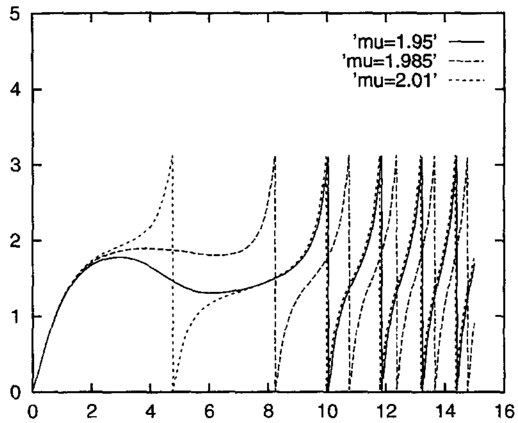

Fig. 1. $c = 0.1$ $\mu = 1.95$, 1.985, 2.01.

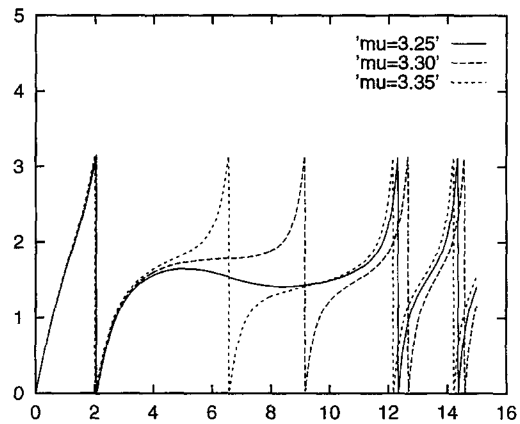

Fig. 2. $c = 0.07$ $\mu = 3.25$, 3.30, 3.35.

depend on μ but change only slightly as μ increases from μ' to μ''. For the same reasons as in [3, (2.18)], we expect the integral in (2.13) to be large and positive – and therefore producing spectral concentration – if

$$(N + \tfrac{1}{2})\pi < \theta(\xi, \mu_0) < (N + 1)\pi \tag{3.1}$$

in (ξ_1, ξ_2), where N ($\geqslant 0$) is an integer. We find that, particularly in situations of sharp concentration, (3.1) is realised with the following features:

(a) $\theta(\xi, \mu')$ and $\theta(\xi, \mu'')$ are close together for $0 \leqslant \xi \leqslant \xi_1$ with their values at ξ_1 close to $(N + \frac{1}{2})\pi$.

(b) $\theta(\xi, \mu'') - \theta(\xi, \mu')$ is close to π for ξ to the right of ξ_2, with $\theta(\xi, \mu'')$ close to $(N + \frac{3}{2})\pi$.

(c) $\theta(\xi_2, \mu_0)$ is close to $(N + 1)\pi$.

Thus the graph of $\theta(\xi, \mu)$ undergoes a rapid transition in (ξ_1, ξ_2) as μ increases from μ' to μ''. This transitional behaviour is identified by our computations and is shown in Figs. 1 and 2. However, it remains an open theoretical question whether this behaviour can be deduced analytically from (2.10) and the nature of R.

4. Computer-assisted investigation of spectral concentration

A computational problem presented by (2.13) is that the infinite integral may converge only slowly, and it is necessary to accelerate the convergence. In the case of (1.7) for example, it follows from (2.2) and (2.4) that $R(\xi,\mu)$ is only $O(\xi^{-1/2})$ as $\xi\to\infty$ and therefore the integral converges only conditionally. However, we can express (2.13) in a more favourable form computationally by using (2.10) to write

$$\begin{aligned}\int_0^\infty R\sin 2\theta\,d\xi &= \int_0^\infty R\sin 2\theta(\theta' - R\sin^2\theta)\,d\xi\\ &= \frac{1}{2}R(0,\mu) + \frac{1}{2}\int_0^\infty R'\cos 2\theta\,d\xi - \int_0^\infty R^2\sin 2\theta\sin^2\theta\,d\xi\end{aligned}$$

after an integration by parts. The two integrals on the right converge more rapidly than the original one, and we can accelerate the convergence further by repeating the integration by parts process. For our purposes in this paper, a suitable form arising from this process is

$$\begin{aligned}\int_0^\infty R\sin 2\theta\,d\xi &= \frac{1}{2}R(0,\mu) - \frac{1}{4}R^2(0,\mu) - \frac{1}{4}\int_0^\infty R''\sin 2\theta\,d\xi\\ &\quad + \int_0^\infty (RR')'\left(\frac{3}{8}\sin 2\theta - \frac{1}{16}\cos 4\theta\right)d\xi\\ &\quad + \int_0^\infty R^2R'\left(\frac{3}{4}\cos 2\theta\sin^2\theta - \frac{1}{4}\cos 4\theta\sin^2\theta - \sin^6\theta\right)d\xi\\ &\quad + \int_0^\infty R^3R'\sin^8\theta\,d\xi + 2\int_0^\infty R^5\sin^9\theta\cos\theta\,d\xi.\end{aligned}$$

The integrals on the right are all $O(\xi^{-5/2})$, or better, as $\xi\to\infty$. Since R is given in terms of x in (2.4), these integrals are evaluated by changing the integration variable back to x, using $d\xi = \{\mu + cs(x)\}^{1/2}\,dx$ by (2.2), the integrands then being $O(x^{-4})$ or better. The integration is then computed over the range $0\leqslant x\leqslant 10^2$, giving a truncation error of order 10^{-6}.

With any chosen value of c, $\rho'(\mu)$ is of course evaluated for a discrete sequence of values of μ, and we have generally taken a mesh size of 10^{-2} for μ. However, as c decreases, we find that spectral concentration becomes very intense and shows itself as a sharp spike in the graph of ρ'. For example, in the next section, we report on a case where the spike has base less than 10^{-2} and height exceeding 2.6×10^5. Of course, once the base is less than the mesh size of 10^{-2}, the spike may be partly or wholly undetected, and therefore the mesh size has to be reduced in order to fully reveal the presence and precise location of the spike. Thus, as c decreases, the mesh size is also decreased in the neighbourhood of the spectral concentration point and we have refined the mesh down to 10^{-6}.

5. The example $q(x) = -cx^2 + x$

We now give the results of our computational procedures for the example (1.7). The unperturbed problem with $q(x) = x$ has a discrete spectrum consisting of positive eigenvalues λ_n $(n = 0,1,\ldots)$.

Table 1

c	$\mu_0(c)$		$\mu_1(c)$		$\mu_2(c)$	
0.26	1.84	(1.58)				
0.2	1.62	(1.76)				
0.15	1.73	(1.90)				
0.12	1.80	(1.99)	2.90	(3.01)		
0.1	1.985	(2.05)	2.86	(3.19)		
0.08	2.06	(2.11)	3.11	(3.37)	3.90	(4.22)
0.07	2.11	(2.14)	3.30	(3.46)	3.92	(4.38)
0.05	2.18	(2.19)	3.58	(3.64)	4.51	(4.71)

The λ_n can be obtained either computationally [2] or analytically in terms of Bessel functions as the zeros of $J_{\frac{1}{3}}(\frac{2}{3}\lambda^{3/2})+J_{-\frac{1}{3}}(\frac{2}{3}\lambda^{3/2})$ [18, Section 4.12]. The first few are

$$\lambda_0=2.34, \qquad \lambda_1=4.09, \qquad \lambda_2=5.52, \qquad \lambda_3=6.79.$$

When $c>0$, the expectation is that there are points of spectral concentration $\mu_n(c)$ such that $\mu_n(c)\to\lambda_n$ as $c\to 0$. This expectation is confirmed by our findings in which c is given a sequence of values starting with $c=0.3$ and decreasing in steps of 0.01. In this sequence $\mu_0(c)$ appears first when $c=0.26$, followed by $\mu_1(c)$ when $c=0.12$ and $\mu_2(c)$ when $c=0.08$. No doubt this process continues. Table 1 gives a selection of our findings, the numbers in brackets being the Titchmarsh approximations (1.9). A refinement of our computations shows that $\mu_0(c)$ and $\mu_1(c)$ first appear for some c in the ranges $(0.263, 0.264)$ and $(0.123, 0.124)$, respectively.

We mention that the sharpness of the spectral concentration increases rapidly as c decreases. In the case of $\mu_0(c)$ for example, we have

$$\rho'(1.6)=0.24, \qquad \rho'(1.73)=4.68, \qquad \rho'(1.85)=1.068$$

when $c=0.15$, showing only moderate sharpness, but when $c=0.1$

$$\rho'(1.98)=24.7, \qquad \rho'(1.985)>2.6\times 10^5, \qquad \rho'(1.99)=10.5.$$

In Figs. 1 and 2 we give graphs of $\theta(\xi,\mu)$, but expressed in terms of x, for values of μ near to $\mu_0(0.1)=1.985$ and $\mu_1(0.07)=3.30$, respectively. The graphs illustrate the transitional nature of θ which was discussed in Section 3 and, of course, the graphs are given mod π. In terms of x, the transitional intervals (x_1,x_2) in which $1+R<0$ are approximately $(2.72, 7.26)$ and $(5.17, 9.10)$, respectively. The graphs also indicate that, if $\mu_0=\mu_n(c)$ in Section 3, it can be conjectured that $N=n$.

Other examples such as $q(x)=-cx^{\alpha}+x^{\beta}$ $(0<\beta<\alpha\leqslant 2)$ are also covered by (2.13) and present a similar picture. We mention however that the proof of the Titchmarsh approximation (1.9) is only valid for $\alpha=2$ and $\beta=1$.

6. Negative discrete unperturbed spectrum

The transformation (2.2) requires $\mu + cs(x) > 0$ for $0 \leqslant x < \infty$. An example such as (1.8) may therefore be excluded because the discrete unperturbed spectrum in $(-\infty, 0)$ leads to the investigation of spectral concentration on $\mu < 0$. This minor difficulty is overcome by a slight modification of (2.2). To accommodate (1.8), we suppose that q has the form (2.1), where s is as before and $p(x) \to 0$ as $x \to \infty$. In (1.1) (with $\lambda = \mu$) we write

$$\mu - q(x) = 1 + cs(x) + \mu - 1 - p(x)$$

and replace (2.2) by

$$\xi = \int_0^x \{1 + cs(t)\}^{1/2}\, dt, \quad \eta = \{1 + cs(x)\}^{1/4} y.$$

Then (2.3), and hence also (2.10) and (2.13), continue to hold but with

$$R(\xi, \mu) = -\frac{1}{4} c \frac{s''(x)}{\{1 + cs(x)\}^2} + \frac{5}{16} c^2 \frac{s'^2(x)}{\{1 + cs(x)\}^3} + \frac{\mu - 1 - p(x)}{1 + cs(x)} \tag{6.1}$$

and the factor $\{\mu + cs(0)\}^{1/2}$ in (2.13) is replaced by $\{1 + cs(0)\}^{1/2}$.

6.1. *Example* $q(x) = -cx - (1 + x)^{-1}$

This is an example of a Stark potential in which $-cx$ represents a weak electric field superimposed on the potential $-(1 + x)^{-1}$, the latter having discrete negative eigenvalues of which the first few are

$$\lambda_0 = -0.12, \qquad \lambda_1 = -0.04, \qquad \lambda_2 = -0.02.$$

Our computational findings are in some respects similar to those in Section 5. However, a new difficulty arises because the values of c which produce spectral concentration are now smaller than before, being no more that 10^{-2} in the case of $\mu_0(c)$ for example. The difficulty is that the term cx in the denominator of R in (6.1) does not begin to dominate the integrand in (2.13) until $x > c^{-1}$ and, with small c, numerical integration over a large range $(0, c^{-1})$ becomes unreliable.

It is possible to give approximate reasoning which indicates the magnitude of c required to produce spectral concentration at a given point μ (<0). In order to have a transition interval in which $R < -1$, it is necessary that the equation $R = -1$ should have two solutions for x. Neglecting the c^2 term in (6.1), the equation is

$$(x + 1)(\mu + cx) + 1 = 0$$

and the condition for real distinct solutions x is

$$c < \mu + 2 - 2\sqrt{(\mu + 1)}.$$

In searching for $\mu_0(c)$ near to $\lambda_0 = -0.12$, the choice $\mu = -0.15$ gives $c < 0.006$ and, for $\mu_2(c)$ near to $\lambda_2 = -0.02$, the choice $\mu = -0.03$ gives $c < 0.00023$. In such circumstances, a computational investigation of spectral concentration on the basis of (2.13) is generally no longer reliable. Of

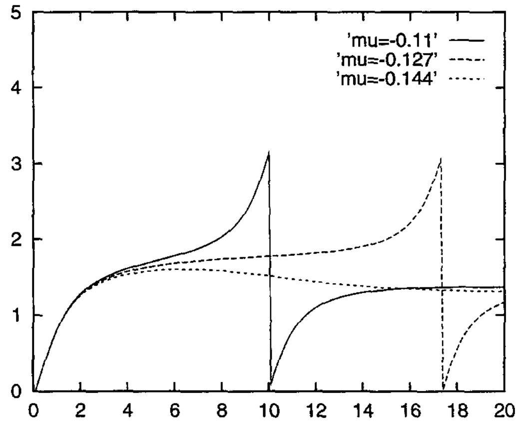

Fig. 3. First point of spectral concentration for $c = 0.001$.

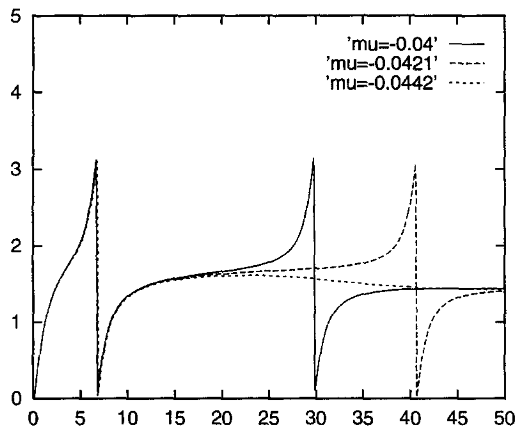

Fig. 4. Second point of spectral concentration for $c = 0.00001$.

course, this difficulty also arises for (1.7) – and indeed for any other such problems – when c is small enough, but (1.8) presents a more extreme case than (1.7). However, the transitional property of the function θ, which was noted in [3] and here in Section 5, provides an alternative albeit indirect method for identifying spectral concentration. This property remains evident for small c and it only requires numerical integration of (2.10) over an interval which includes the transition interval. Figs. 3–5 show the transitional property of θ for $\mu_0(10^{-3})$, $\mu_1(10^{-5})$, $\mu_2(2 \times 10^{-6})$. Once again the figures lead to the conjecture that, if $\mu_0 = \mu_n(c)$ in Section 3, then $N = n$.

There does nevertheless remain one situation where direct computation of ρ' is possible on the basis of (2.13) and (6.1). In the case of $\mu_0(c)$ spectral concentration rapidly becomes intense for only moderately small values of c (as in Section 5). Consequently, when μ is near to $\mu_0(c)$, we are able to integrate in (2.13) over a long x-interval $(0, 5000)$ because the signal/noise ratio is large. That is, the accumulated errors in the numerical integration remain small in relation to the actual value of the integral. On this basis, Table 2 gives the spectral concentration points for Example 6.1,

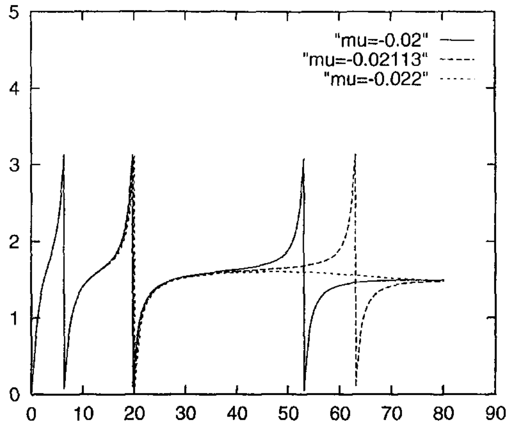

Fig. 5. Third point of spectral concentration for $c = 0.000001$.

Table 2

c	$\mu_0(c)$	$\mu_1(c)$	$\mu_2(c)$
0.033	−0.188		
0.02	−0.204		
0.01	−0.181		
0.005	−0.152	−0.12	
0.001	−0.127	−0.0625	
0.0005	−0.125	−0.051	−0.040
0.0001	−0.123	−0.0435	−0.024
0.00001	−0.122	−0.0421	−0.021

where the entries for $\mu_0(c)$ $(0.001 \leqslant c \leqslant 0.033)$ are derived from (2.13) and all the other entries are derived from the transitional properties of θ. The value 0.033 for c is included because it is the first value for which $\mu_0(c)$ appears.

We conclude by recalling the theoretical questions to which our computational findings draw attention. These questions are those stated at the end of Sections 1 and 3 and, concerning $N = n$, in this section and at the end of Section 5.

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