Available online at www.sciencedirect.com
ScienceDirect
JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS
Journal of Computational and Applied Mathematics 212 (2008) 150 – 178
www.elsevier.com/locate/cam

Efficient calculation of spectral density functions for specific classes of singular Sturm–Liouville problems☆

Charles Fulton[a,*], David Pearson[b], Steven Pruess[c]

[a]Department of Mathematical Sciences, Florida Institute of Technology, Melbourne, FL 32901-6975, USA
[b]Department of Mathematics, University of Hull, Cottingham Road, Hull, HU6 7RX England, UK
[c]1133 N Desert Deer Pass, Green Valley, AZ 85614-5530, USA

Received 3 January 2006; received in revised form 24 October 2006

Abstract

New families of approximations to Sturm–Liouville spectral density functions are derived for cases where the potential function has one of several specific forms. This particular form dictates the type of expansion functions used in the approximation. Error bounds for the residuals are established for each case. In the case of power potentials the approximate solutions of an associated terminal value problem at ∞ are shown to be asymptotic power series expansions of the exact solution. Numerical algorithms have been implemented and several examples are given, demonstrating the utility of the approach.

MSC: 65L15

Keywords: Sturm–Liouville problem; Spectral density function; Spectral function; Terminal value problem; Asymptotic power series; Step function approximation

1. Introduction

In this paper we extend the analysis in [7] to specific classes of potentials, for which iteration schemes yielding recurrence relations for high order approximations for the solution of the terminal value problem of [7, Section 1] can be obtained. The Sturm–Liouville problem considered is

$$-u'' + qu = \lambda u, \quad a \leqslant x < \infty, \tag{1.1}$$

$$u(a)\cos\alpha + u'(a)\sin\alpha = 0, \quad \alpha \in [0, \pi], \tag{1.2}$$

under the assumptions

$$q \in L_1[a, \infty), \tag{1.3}$$

☆ This research partially supported by National Science Foundation Grant DMS-0109022 to Florida Institute of Technology, and by EPSRC Grant S63403/01 to University of Hull.
* Corresponding author. Tel.: +1 321 674 7218; fax: +1 321 984 8461.
E-mail address: cfulton@fit.edu (C. Fulton).

0377-0427/$ - see front matter
doi:10.1016/j.cam.2006.11.030

or

$$q' \in L_1(a,\infty), \quad q \in AC_{\mathrm{loc}}[a,\infty), \quad \lim_{x\to\infty} q(x) = 0. \tag{1.4}$$

Under these assumptions, Corollary 1 or Corollary 2 of [7] apply to ensure existence and uniqueness of solutions of the terminal value problem for P, Q, R. Letting $y(x,\lambda) = y_\alpha(x,\lambda)$ be the solution of (1.1) fixed by the initial conditions

$$y_\alpha(a,\lambda) = -\sin\alpha, \quad y'_\alpha(a,\lambda) = \cos\alpha \tag{1.5}$$

we seek functions $P_N(x,\lambda)$, $Q_N(x,\lambda)$, $R_N(x,\lambda)$, $N \to \infty$, satisfying the terminal conditions at ∞ ((2.2) below), and for which

$$F_x^N(\lambda) := \frac{1}{\pi[P_N(x,\lambda)y(x,\lambda)^2 + Q_N(x,\lambda)y(x,\lambda)y'(x,\lambda) + R_N(x,\lambda)y'(x,\lambda)^2]} \tag{1.6}$$

gives increasingly more accurate approximations to the spectral density function $f(\lambda)$ as $N \to \infty$.

In [6] we took the constant values $P(x,\lambda) = \sqrt{\lambda}$, $Q(x,\lambda) = 0$, and $R(x,\lambda) = 1/\sqrt{\lambda}$, corresponding to the classical formula of Titchmarsh and Weyl, and demonstrated numerically the efficacy of this choice when x was chosen sufficiently large. In [7] we improved on this by deriving a sequence of more sophisticated formulas for P, Q, R in terms of the general potential q and its derivatives; these usually allowed smaller values of x to be used for a given accuracy compared to the methods in [6], but did not take advantage of special forms of q. In this paper we assume q takes on one of the following special forms:

- decaying exponential: $q(x) = A\exp(-\alpha x)$ for some $\alpha > 0$. The difficult examples are when $\alpha \approx 0$;
- power function: $q(x) = A/x^E$ for E a positive rational number;
- product of a power and a trigonometric function: $q(x) = [A\cos\omega x + B\sin\omega x]/x^E$ for E a positive integer.

The latter class includes many examples that occur in the study of resonances and gives rise to points of spectral concentration [4].

In the next section we summarize the theoretical results from [7] that are being utilized in this paper. In Section 3 we obtain general error bounds for the approximate solutions in terms of the residuals defined by (2.5) below. In Sections 4 and 5 we derive the approximation formulas and recurrence relations for slowly decaying exponential functions, and power potentials with E a positive integer. In Section 6 we prove that the approximate solutions in the case of power potentials are asymptotic power series expansions of the exact solution of the terminal value problem (2.1)–(2.2) below. In Sections 7 and 8 we derive the approximate solutions and recurrence relations for power potentials with E rational, and products of power potentials with trigonometric functions. In Section 9 some numerical examples for each class of potential are given, and in Section 10 come clues for possible generalization of the basic method to other classes of problems are given. Our numerical experience for the cases of slowly decaying exponential functions, power potentials with positive rational E, and products of power and trigonometric functions is that we retain convergence of F_x^N to f for fixed N as $x \to \infty$, but that for fixed x, F_x^N is divergent as $N \to \infty$; in other words, the behavior is similar to the case of asymptotic power series for the power potentials when N a positive integer. The main advantage of adapting the approximate solutions to the given form of potential is that the values of x needed for a given accuracy can be much smaller than those for the methods in [6,7].

2. Mathematical background

In this section the theory of [7] is reviewed, showing that it is sufficiently general to cover the new approximations obtained for our specific classes of potentials. First, taking the residual terms to be exactly zero in the first order linear system for P, Q, R we seek functions $P(x,\lambda)$, $Q(x,\lambda)$, and $R(x,\lambda)$ satisfying the differential equations

$$\begin{aligned} P' &= (\lambda - q(x))Q, \\ Q' &= -2P + 2(\lambda - q(x))R, \\ R' &= -Q, \end{aligned} \tag{2.1}$$