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Numerical computation and analysis of the Titchmarsh–Weyl $m_\alpha(\lambda)$ function for some simple potentials

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Abstract

This article is concerned with the Titchmarsh–Weyl $m_\alpha(\lambda)$ function for the differential equation $\mathrm{d}^2y/\mathrm{d}x^2+[\lambda-q(x)]y=0$. The test potential $q(x)=x^2$, for which the relevant $m_\alpha(\lambda)$ functions are meromorphic, having simple poles at the points $\lambda=4k+1$ and $\lambda=4k+3$, is studied in detail. We are able to calculate the $m_\alpha(\lambda)$ function both far from and near to these poles. The calculation is then extended to several other potentials, some of which do not have analytical solutions. Numerical data are given for the Titchmarsh–Weyl $m_\alpha(\lambda)$ function for these potentials to illustrate the computational effectiveness of the method used.

1. Introduction

The purpose of this work is to test and apply a method for calculating the Titchmarsh–Weyl $m_\alpha(\lambda)$ function for the second order differential equation

$$-\frac{\mathrm{d}^2y}{\mathrm{d}x^2}+q(x)y=\lambda y. \tag{1}$$

Several potentials are treated, some with and some without analytical solutions. We first check the accuracy of the method by studying the test case $q(x)=x^2$, for which $m_\alpha(\lambda)$ has a known analytical form in terms of special functions. We succeed in calculating $m_\alpha(\lambda)$ to high accuracy even close to the poles, a region which has not previously been explored in detail by numerical methods; comparative calculations show that some previously proposed methods [4] are not so accurate in this region. The high accuracy enables us to establish some numerical details about the formal spectral sum expression for the $m_\alpha(\lambda)$ function and to establish various relationships which are not readily available in the previous literature.

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The concept of the $m_\alpha(\lambda)$ function arose in the classic work of Weyl [12], in which he considered the square-integrable solutions of equation (1) on the half-open interval $[0,\infty)$, where $q(x)$ is real-valued and locally Lebesgue integrable in $[0,\infty)$ and λ is a complex number. Eq. (1) is said to be of limit-circle type if all solutions of it are $L^2(0,\infty)$; if there is a solution which is not $L^2(0,\infty)$ for $\operatorname{Im}\lambda \neq 0$, the equation is said to be limit-point. Weyl's classification of Eq. (1) into limit-point and limit-circle types has important consequences for the spectral theory associated with Eq. (1) in the Hilbert space $L^2(0,\infty)$, as further shown by Titchmarsh [9–11], who considered the analytic properties of the square-integrable solutions of the differential equation and their relationship with the $m_\alpha(\lambda)$ function.

The analytic form for $m_\alpha(\lambda)$ is known in those few cases where the closed analytic form of the square-integrable solutions can be found. For example, when $q(x)$ is a positive power of x, the only known examples are $q(x)=x^2$, for which the $m_\alpha(\lambda)$ function is a quotient of gamma functions, and $q(x)=x$, for which the $m_\alpha(\lambda)$ function involves a quotient of sums of Bessel functions. In view of the difficulty of finding the $m_\alpha(\lambda)$ function in closed form, numerical approaches to calculating $m_\alpha(\lambda)$ have been developed [2–4,8].

The results reported in this work were obtained by simply using the differential equation solver NDSolve of the widely available Mathematica package. This solver uses an adaptive steplength approach to maintain accuracy throughout the integration region. It emerges from our calculations that this solver is highly effective even for a specialized task such as the calculation of the $m_\alpha(\lambda)$ function and that it even compares favourably with some of the specialized programs specifically designed to treat the $m_\alpha(\lambda)$ function.

2. Analytical properties of $m_\alpha(\lambda)$ for $q(x)=x^2$

In this paper we use the real potential $q(x)=x^2$ to provide a test case for our computational method. The analytic solutions to Eq. (1) involve Hermite polynomials, and arise in the quantum theory of the harmonic oscillator. The equation to be studied is

$$\frac{d^2y}{dx^2}+[\lambda-x^2]y=0, \tag{2}$$

which for $-\infty<x<+\infty$ has a discrete spectrum; λ is taken to be complex and is written as $\lambda=u+iv$. It is known that the parabolic cylinder functions $D_n(z)$ of harmonic analysis [9] obey Weber's equation

$$\frac{d^2y}{dz^2}+\left[n+\frac{1}{2}-\frac{1}{4}z^2\right]y=0. \tag{3}$$

The change of variable $z=\sqrt{2}x$, transforms equation (3) to the form

$$\frac{d^2y}{dx^2}+[2n+1-x^2]y=0. \tag{4}$$

The equations (2) and (4) are the same if $\lambda=(2n+1)$, i.e., $n=(\lambda-1)/2$. Hence a solution of Eq. (2) for the λ value $\lambda=2n+1$ is

$$y=D_n(\sqrt{2}x); \quad n=(\lambda-1)/2. \tag{5}$$

This result is valid even when λ is complex and enables analytical results for the $m_\alpha(\lambda)$ function for $q(x) = x^2$ to be obtained in terms of gamma functions. For the case $x \in [0,\infty)$, with λ complex, we denote by $\theta(x,\lambda)$ and $\phi(x,\lambda)$ the solutions of the differential Eq. (4) which satisfy the initial conditions

$$\theta(0,\lambda) = \sin\alpha, \qquad \theta'(0,\lambda) = -\cos\alpha, \tag{6}$$

$$\phi(0,\lambda) = \cos\alpha, \qquad \phi'(0,\lambda) = \sin\alpha \tag{7}$$

for some $\alpha \in [0,\pi]$, where prime denotes differentiation with respect to x. The analytic function $m_\alpha(\lambda)$, unique in the limit point case, is holomorphic in the upper and lower half-planes and is such that the solution ψ of Eq. (4) defined by

$$\psi(x,\lambda) = \theta(x,\lambda) + m_\alpha(\lambda)\phi(x,\lambda) \quad (x \in [0,\infty)) \tag{8}$$

has the property $\psi(x,\lambda) \in L^2[0,\infty)$, i.e.

$$\int_0^\infty |\theta(x,\lambda) + m_\alpha(\lambda)\phi(x,\lambda)|^2\,\mathrm{d}x < \infty. \tag{9}$$

From Eqs. (6), (7) and (9), we obtain ψ and ψ' at the origin:

$$\psi(0,\lambda) = \sin\alpha + m_\alpha(\lambda)\cos\alpha, \tag{10}$$

$$\psi'(0,\lambda) = -\cos\alpha + m_\alpha(\lambda)\sin\alpha. \tag{11}$$

Let

$$\psi(x,\lambda) = C(\lambda)D_n(\sqrt{2}x), \qquad n = (\lambda-1)/2, \quad \lambda = u + \mathrm{i}v. \tag{12}$$

We now consider the two cases, $\alpha = 0$ and $\alpha = \pi/2$, in turn. When $\alpha = 0$ we have

$$\theta(0) = 0, \qquad \theta'(0) = -1, \qquad \phi(0) = 1, \qquad \phi'(0) = 0. \tag{13}$$

Therefore

$$m_0(\lambda) = -\frac{\psi(0,\lambda)}{\psi'(0,\lambda)} = -\frac{D_n(0)}{\sqrt{2}D_n'(0)}, \tag{14}$$

where $D_n(0)$ and $D_n'(0)$ can be given [1] as

$$D_n(0) = -\frac{2^{n/2}\sqrt{\pi}}{\Gamma(\frac{1}{2}-\frac{1}{2}n)}, \tag{15}$$

$$D_n'(0) = -\frac{2^{n/2+1/2}\sqrt{\pi}}{\Gamma(-\frac{1}{2}n)}. \tag{16}$$

Eqs. (14)–(16) give

$$m_0(\lambda) = \frac{\Gamma(-\frac{1}{2}n)}{2\Gamma(\frac{1}{2}-\frac{1}{2}n)} \tag{17}$$

while setting $n = (\lambda-1)/2$ in Eq. (17), gives

$$m_0(\lambda) = \frac{\Gamma(\frac{1}{4}-\frac{1}{4}\lambda)}{2\Gamma(\frac{3}{4}-\frac{1}{4}\lambda)}. \tag{18}$$

The function $m_0(\lambda)$ has poles at the points

$$\lambda=(4n-3), \qquad n=1,2,\dots \tag{19}$$

because $\Gamma(n)$ has a pole at $n=0$, and at all negative integer values of n.

For the test case $q(x)=x^2$, setting $\lambda, \lambda+2$ and $\lambda-2$ in turn in Eq. (18) and using the property $z\Gamma(z)=\Gamma(z+1)$ produces the relationships

$$(\lambda-1)m_0(\lambda-2)=(\lambda+1)m_0(\lambda+2)=-\frac{1}{m_0(\lambda)} \tag{20}$$

and our independent numerical results were found to satisfy these relations to high accuracy for the case $q(x)=x^2$.

In the case $\alpha=\frac{1}{2}\pi$, the initial conditions (8) and (9) for θ and ϕ are

$$\theta(0,\lambda)=0, \quad \theta'(0,\lambda)=-1, \quad \phi(0,\lambda)=1, \quad \phi'(0,\lambda)=0. \tag{21}$$

We then find

$$m_{\pi/2}(\lambda)=\frac{\psi'(0,\lambda)}{\psi(0,\lambda)}=\left\{\sqrt{2}\frac{D_n'(0)}{D_n(0)}\right\}=-\frac{2\Gamma(\frac{3}{4}-\frac{1}{4}\lambda)}{\Gamma(\frac{1}{4}-\frac{1}{4}\lambda)}. \tag{22}$$

The eigenvalues are given by $\lambda=(4n-1)$, $n=1,2,3,\dots$.

3. Numerical calculation of the function $m_\alpha(\lambda)$

Much research has been done on the Titchmarsh–Weyl m-coefficient, but so far theoretical studies far outnumber numerical studies, which are principally represented by the works [2–4,8]. In the present work, extensive analysis of some analytical and numerical calculations of the m-coefficient is presented.

All the computational algorithms which have been used to calculate the Titchmarsh–Weyl m-coefficient associated with the second order differential equation

$$-\psi''(x)+x^2\psi(x)=\lambda\psi(x) \tag{23}$$

are based on approaches which involve integrating Eq. (23) over the region $0\leqslant x\leqslant X$ and looking at the limit $X\to\infty$. There are two obvious ways to perform an integration over the x region considered:

1. Start at a large x value, $x=X$, with $\psi(X)=0$, $\psi'(X)=1$ and integrate Eq. (23) for ψ backwards to $x=0$, forming the ratio $-\psi(0)/\psi'(0)$. As X is increased this computed ratio tends towards its asymptotic value $m_0(\lambda)$.
2. Start at $x=0$, using two functions u and v, with $v(0)=u'(0)=1$, $u(0)=v'(0)=0$. Integrate forwards to $x=X$ and form the ratio $-v(X)/u(X)$. As X is increased this ratio will tend towards the function $m_0(\lambda)$. Combining Eqs. (18) and (22) shows that

   $$m_0(\lambda)=-\frac{1}{m_{\pi/2}(\lambda)} \tag{24}$$

   and so, in principle, the result of either forwards or backwards integration can be used to give both $m_0(\lambda)$ and $m_{\pi/2}(\lambda)$, although in practice one or other of the methods may be more accurate for a particular λ value.

In the calculations reported here we utilized Mathematica's built-in differential equation solver. In principle X should be 'sufficiently close' to infinity when we integrate backwards from X using the appropriate initial values. In fact, for the case of a test potential which grows rapidly with x, the X value can often be taken to be fairly small to give a required level of accuracy, e.g. $X=5$ is often adequate for $q(x)=x^2$.

In this work, we cross-checked the accuracy of the numerical $m_\alpha(\lambda)$ estimates produced by our Mathematica [14] code by using various alternative numerical routines to calculate $m_\alpha(\lambda)$. Where the exact analytic form is known, we give the true value to 25 places, and our calculated values agree with the true value to 22 digits; in our numerical comparisons we used the Kirby code [8] with an absolute tolerance of $\mathrm{TOL}=10^{-11}$–10^{-14} as one of the alternative methods.

Setting $\lambda = 4n-1 \pm i\lambda_{\mathrm{I}}$ in the first two members of Eq. (20) gives the ratio

$$r_0 = \frac{m_0(4n+1 \mp i\lambda_{\mathrm{I}})}{m_0(\lambda = 4n-3 \mp i\lambda_{\mathrm{I}})} = \frac{4n-2 \mp i\lambda_{\mathrm{I}}}{4n \mp i\lambda_{\mathrm{I}}} \tag{25}$$

which will be required in our later analysis.

4. Parameterizations of Titchmarsh–Weyl $m_\alpha(\lambda)$ functions at poles

If $m_\alpha(z)$ is analytic in the upper half plane, maps the upper half plane to itself and satisfies the Herglotz condition

$$\operatorname{Im} m_\alpha(z) > 0 \quad \text{if } \operatorname{Im} z > 0 \tag{26}$$

then it is known that $m_\alpha(z)$ can be represented in the form [5,6]

$$m_\alpha(z) = C_1 + C_2 z + \int_{-\infty}^{\infty} \left[\frac{1}{\lambda - z} - \frac{\lambda}{\lambda^2+1}\right] \mathrm{d}\rho_\alpha(\lambda), \tag{27}$$

where C_1 and C_2 are uniquely determined real constants with $C_2 \geqslant 0$, while the spectral function $\rho_\alpha(\lambda_n)$ is locally bounded, non-decreasing right-continuous and satisfies the convergence condition

$$\int_{-\infty}^{\infty} \frac{\mathrm{d}\rho_\alpha(\lambda)}{\lambda^2+1} < \infty. \tag{28}$$

The spectral density $\mathrm{d}\rho_\alpha(\lambda)/\mathrm{d}\lambda$ is given almost everywhere by

$$\frac{\mathrm{d}\rho_\alpha(\lambda)}{\mathrm{d}\lambda} = \lim_{\delta\to 0+} \frac{1}{\pi} \operatorname{Im}[m_\alpha(\lambda + \mathrm{i}\delta)]. \tag{29}$$

In quantum mechanical applications to the Schrödinger equation, the spectral density may be thought of as a local probability density for the energy of the system. Mathematically, the spectral density provides a complete description of the absolutely continuous spectrum.

In the case of the discrete spectrum for $q(x)=x^2$, the functions $m_0(\lambda)$ and $m_{\pi/2}(\lambda)$ are meromorphic, and the spectral function ρ is a step function on $\mathbb{R}$. The spectrum of the differential operator in $L^2(0,\infty)$, subject to Neumann and Dirichlet boundary condition respectively, consists of poles (eigenvalues) at $\lambda=(4K+1)$ and $\lambda=(4K+3)$ for $K=0,1,2,\ldots$.

For $\alpha = 0$, the corresponding $m_0(z)$ can then be expressed as a sum

$$m_0(z) = \int_{-\infty}^{\infty} \frac{1}{\lambda - z}\, \mathrm{d}\rho(\lambda) \equiv \sum_{K=0}^{\infty} \frac{C_{4K+1}}{(4K+1) - z}. \tag{30}$$

Setting $z = 4J + 1 + \mathrm{i}\beta$ with $\beta \to 0$ allows us to extract the coefficient C_{4J+1}. At $z = 4J + 1 + \mathrm{i}\beta$, the $m_0(z)$ function has the real and imaginary parts

$$\mathrm{Re}\, m_0(4J + 1 + \mathrm{i}\beta) = \sum_{\substack{K=0 \\ K \neq J}}^{\infty} \frac{4(K - J)C_{4K+1}}{[4K - 4J]^2 + \beta^2} = 0 + S_1(\beta), \tag{31}$$

$$\mathrm{Im}\, m_0(4J + 1 + \mathrm{i}\beta) = \frac{C_{4J+1}}{\beta} + \sum_{\substack{K=0 \\ K \neq J}}^{\infty} \frac{C_{4K+1}\beta}{[4K - 4J]^2 + \beta^2} \equiv \frac{C_{4J+1}}{\beta} + S_2(\beta), \tag{32}$$

Table 1
Analytic values of the Titchmarsh–Weyl function $m_0(\lambda) = \Gamma((1-\lambda)/4)/[2\Gamma(3-\lambda)/4)]$, for $\lambda = \lambda_R + i\lambda_I \equiv 4n - 3 + i10^{-12}$ and of $m_{\pi/2}(\lambda) = -2\Gamma((3-\lambda)/4)/(2\Gamma((1-\lambda)/4))$ for $\lambda = \lambda_R + i\lambda_I \equiv 4n - 1 + i10^{-12}$, over a wide range of values of the quantum number n, for the case $q(x) = x^2$

n	$\mathrm{Re}\, m_0(\lambda)$	$\mathrm{Im}\, m_0(\lambda)$
1	0.3910664191374169765549597954 5	$1.1283791670955125738961589 51 \times 10^{12}$
2	0.0544858136817694165404600498 4	$5.6418958354775628694807955 98 \times 10^{11}$
3	0.0232334357754596784382175516 2	$4.2314218766081721521105967 37 \times 10^{11}$
4	0.0134842216509272707094721309 5	$3.5261848971734767934254972 89 \times 10^{11}$
5	0.0090438619936445831259244448 4	$3.0854117850267921942473101 31 \times 10^{11}$
6	0.0065967699017667287162083453 0	$2.7768706065241129748225791 19 \times 10^{11}$
7	0.0050828478937986287624886987 7	$2.5454647226471035602540308 59 \times 10^{11}$
8	0.0040704340843826288610216409 9	$2.3636458138865961630930286 56 \times 10^{11}$
9	0.0033543823810839887441036812 7	$2.2159179505186839028997143 65 \times 10^{11}$
10	0.0028260651576721183967615455 2	$2.0928113977120903527386191 22 \times 10^{11}$
11	0.0024231604750745011828311408 6	$1.9881708278264858351016881 66 \times 10^{11}$
12	0.0021076272687873868899026914 6	$1.8977994265616455698697932 50 \times 10^{11}$
13	0.0018550699323655473693277708 8	$1.8187244504549103377918851 98 \times 10^{11}$
14	0.0016492000495781956703749361 1	$1.7487735100527984017229665 36 \times 10^{11}$
15	0.0014787711249725459269353359 3	$1.6863173132651984588042891 60 \times 10^{11}$
16	0.0013357944589587278149928086 7	$1.6301067361563585101774795 21 \times 10^{11}$
17	0.0012144558266398828778945236 6	$1.5791659006514723067344332 86 \times 10^{11}$
18	0.0011104335142364835412291815 6	$1.5327198447499584153598911 31 \times 10^{11}$
19	0.0010204554287812278867135603 4	$1.4901442935069040149332274 88 \times 10^{11}$
20	0.0009420035444536434958259033 7	$1.4509299699935644355928793 96 \times 10^{11}$
21	0.0008731118942800035198179783 1	$1.4146567207437253247030574 12 \times 10^{11}$
250	0.0000202225929083115539456460 9	$4.0323890825896471203816892 42 \times 10^{10}$
251	0.0000201014999408431378953471 7	$4.0243243044244678261409258 63 \times 10^{10}$
250 000	0.0000000006366226371665042103 8	$1.2732414545984586708280479 94 \times 10^{9}$
250 001	0.0000000006366188174383206804 5	$1.2732389081155494739107063 37 \times 10^{9}$
2 500 001	0.0000000000201316818220422135 7	$4.0263367670421194178725317 73 \times 10^{8}$
2 500 002	0.0000000000201316697430403677 4	$4.0263359617750881162611688 43 \times 10^{8}$

Table 1a
(*Contd.*)

n	$-\mathrm{Re}\, m_{\pi/2}(\lambda)$	$\mathrm{Im}\, m_{\pi/2}(\lambda)$
1	0.346246328820678620786239360 45	$2.25675833419102514779231829 3 \times 10^{12}$
2	0.23727470145713978770531926076	$3.38513750128653772168847741 3 \times 10^{12}$
3	0.19080782990622043082888415751	$4.23142187660817215211059676 0 \times 10^{12}$
4	0.16383938660436588940993989560	$4.93665885604286751079569621 8 \times 10^{12}$
5	0.14575166261707672315809100591	$5.55374121304822594964515824 5 \times 10^{12}$
6	0.13255812281354326572567431531	$6.10911533435304854460967406 9 \times 10^{12}$
7	0.12239242702594600820069691775	$6.61820827888246925666048024 0 \times 10^{12}$
8	0.11425155885718075047865363576	$7.09093744165978848927908597 2 \times 10^{12}$
9	0.10754279409501277299044627322	$7.53412103176352526985902884 5 \times 10^{12}$
10	0.10189066377966853619692318216	$7.95268331130594334040675266 9 \times 10^{12}$
11	0.09704434282951953383126090043	$8.35031747687124050742709030 3 \times 10^{12}$
12	0.09282908829194476005145551749	$8.72987736218356962140104895 3 \times 10^{12}$
13	0.08911894842721366531279997573	$9.09362225227455168895942599 2 \times 10^{12}$
14	0.08582054832805727397205010350	$9.44337695428511136930401930 0 \times 10^{12}$
15	0.08286300607811218211817943163	$9.78064041693815106106487713 2 \times 10^{12}$
16	0.08019141716019472648819381427	$1.01066617641694227631003730 3 \times 10^{13}$
17	0.07776250550691496073240476695	$1.04224949442997172244472596 9 \times 10^{13}$
18	0.07554163847844199364994640383	$1.07290389132497089075192379 2 \times 10^{13}$
19	0.07350072762087953787651928313	$1.10270677719510897105058834 1 \times 10^{13}$
20	0.07161672053197225088486747638	$1.13172537659498025976244592 9 \times 10^{13}$
21	0.06987049674341224384523151976	$1.16001851100985476625650707 7 \times 10^{13}$
250	0.02014174310340154036606208826	$4.02432430442446782614092586 3 \times 10^{13}$
251	0.02010154010351985409027139392	$4.03237295303331676179320771 4 \times 10^{13}$
250 000	0.00063662009067722879345685121	$1.27323890811554947391070633 7 \times 10^{15}$
250 001	0.00063661881743959391681549030	$1.27324145459336570500965415 8 \times 10^{15}$
2 500 000	0.00020131685848378980610382104	$4.02633676704211941787253177 3 \times 10^{15}$
2 500 001	0.00020131681822042616201939390	$4.02633757230947282629641534 7 \times 10^{15}$

where $S_1(\beta)$ and $S_2(\beta)$ are infinite series in even and odd positive powers of β, respectively. Our integrator was found to be capable of computing $m_0(\lambda)$ even at points very close to the poles, where it tends to infinity. This thus made it possible to find the residues C_{4J+1} directly from Eq. (32) by using the sufficiently small probe value $\beta = 10^{-12}$ and computing $\mathrm{Im}\, m_0(4J+1+\mathrm{i}\beta)$. In this way we obtained the numerical value $C_1 = 1.1283791670955125738961589 51$ together with a long sequence of C_{4K+1} values which obeyed the law

$$\frac{C_{4K+1}}{C_{4K+5}} = \frac{2K+2}{2K+1} \tag{33}$$

to extremely high accuracy. This result, which does not appear to have been given in the previous literature, was initially conjectured solely on the basis of our numerical calculation, which involves using Eq. (32) and approaching each pole by decreasing the imaginary part of λ. As pointed out by the referee, one can derive this result analytically. Setting $n = K + 1$ in Eq. (25) and taking the limit $\lambda_{\rm I} \to 0$ yields Eq. (33) directly; even though both of the $m_0(\lambda)$ functions in Eq. (25) then have a pole at $\lambda_{\rm I} = 0$, their ratio correctly gives the ratio of the residues at these poles. The leading coefficient C_1 equals -1 times the residue of $m_0(\lambda)$ at $\lambda = 1$. Setting $\lambda = 1 + \varepsilon$ in Eq. (18) gives

$$C_1 = \lim_{\varepsilon \to 0} 2 \left[\frac{-\frac{\varepsilon}{4}\Gamma(-\frac{\varepsilon}{4})}{\Gamma(\frac{1}{2} - \frac{\varepsilon}{4})} \right]. \tag{34}$$

From the property $z\Gamma(z) = \Gamma(z+1)$ it follows that as $\varepsilon \to 0$ the bracketed quantity in the numerator gives in the limit $\Gamma(1) = 1$. The denominator gives $\Gamma(\frac{1}{2}) = \sqrt{\pi}$, leading to the result $C_1 = 2/\sqrt{\pi}$, which agrees to all digits with our computed C_1 value. This a posteriori analysis indicates the numerical accuracy of our computations of the m-function even near a pole. For a more general $q(x)$ there will be no such rational number ratio such as that of Eq. (33) between the C_K coefficient associated with the poles. The sum in Eq. (31) converges very slowly indeed. For example, taking even 10^7 terms, with the C_K as given by Eq. (33), we find $\operatorname{Re} m_0(1 + {\rm i}10^{-12}) = 0.390965$, whereas the truncated analytical result is $\operatorname{Re} m_0(1 + {\rm i}10^{-12}) = 0.391066$.

5. Numerical results and discussion

The Mathematica Code [14] gives results which compare favourably with those of more specialized codes [8], particularly near poles of the $m_\alpha(\lambda)$ function. The accuracy of our results permitted the discovery or verification of various relationships which link values of $m_0(\lambda)$ and $m_{\pi/2}(\lambda)$ even at different $\lambda_{\rm R}$ values and which are computationally useful. It also led to the formula (33), relating the coefficients C_N in the spectral sum formalism, which had not previously been studied computationally. The poles of the functions $m_0(\lambda)$ and $m_{\pi/2}(\lambda)$ can be regarded as the real eigenvalues of an associated boundary value problem with Neumann or Dirichlet boundary conditions at the regular endpoint. This fact enables the pole positions to be found by a shooting process for more complicated potentials $q(x)$. We found that the Mathematica Code [14] is also highly accurate for this auxiliary task, as confirmed by comparison with the method of [7] for several test cases.

Tables 1 and 1a shows some $m_0(\lambda)$ and $m_{\pi/2}(\lambda)$ values at points very close to the poles over a wide range of values of state number $n\,(1 \leqslant n \leqslant 250002)$. It is clear that $\operatorname{Re} m_\alpha(\lambda)$ is very small compared to $\operatorname{Im} m_\alpha(\lambda)$ in these regions.

Table 2 shows $m_\alpha(\lambda)$ for different index values K of the imaginary part $\lambda_{\rm I} = 10^K = -9 \leqslant K \leqslant 8$ for $\lambda = (1 + {\rm i}10^K$ and $3 + {\rm i}10^K)$ very close to the $\alpha = 0$ and $\alpha = \pi/2$ poles, respectively. We note that as the value of K changes from 1 to 8 we find $\operatorname{Re} m_\alpha(\lambda) \simeq \operatorname{Im} m_\alpha(\lambda)$, but when K changes from -1 to -9 the real part is almost constant while the imaginary part increases by a factor of 10 as the index K changes by -1. This is in accord with the spectral sum representation (30) of the $m_\alpha(\lambda)$ functions.

Table 3 shows $m_\alpha(\lambda)$ values at $\lambda_{\rm R} \pm {\rm i}10^{-N} (\lambda_{\rm R} = 1, 3;\ N = 5, 9)$. We observed marked differences in the behaviour of $m_\alpha(\lambda)$ at $\lambda_{\rm R} \pm {\rm i}10^{-N}$ and at $\lambda_{\rm R}$; we deliberately choose these critical points in order to understand the typical features of their behaviour. For example at $Z = 1 \pm 10^{-9} + {\rm i}10^{-9}$

Table 2
Values of the Titchmarsh–Weyl function $m_0(\lambda = 1 + \mathrm{i}10^K)$ and $m_{\pi/2}(\lambda = 3 + \mathrm{i}10^K)$ for $-9 \leqslant K \leqslant 8$, with $q(x) = x^2$. The full results are analytical calculations; the underlined digits show the accuracy of our numerical calculations

X, No.	K	$\mathrm{Re}\, m_0(\lambda = 1 + \mathrm{i}10^K)$	$\mathrm{Im}\, m_0(\lambda = 1 + \mathrm{i}10^K)$
	8	0.00007071067776510136096292717	0.0000707106784722081421494747440
	7	0.00022360678656963880263340182	0.0002236068089303185776314385385
	6	0.00070710642763306854255846285	0.0007071071347398497295479289971
	5	0.00223605679713195064896703238	0.0022360791578117270444064831115
	4	0.00707071424963383738060326965	0.0070714213564194433457305048946
	3	0.02234949663303401029153879206	0.0223718573267845027511667994716
8 8000	2	0.07035621862039376656445574060	0.0710633696178231998887229073869
8 8000	1	0.21206913372094869804031448142	0.2345777326670125989999425143289
10 9000	0	0.38158898413911704906907013733	$0.117441835220918644394663802 \times 10^1$
8 6000	−1	0.39096637013407974412977764126	$0.112886133586577323189099487 \times 10^2$
10 10^4	−2	0.39106541808764829366940620579	$0.112838399109086980343834798 \times 10^3$
9 9000	−3	0.39106640912686328191804043455	$0.112837921533569704965760896 \times 10^4$
8 8000	−4	0.39106641903731143400777550704	$0.112837916757791444174425809 \times 10^5$
8 9000	−5	0.39106641913641592112892788093	$0.112837916710033659257694894 \times 10^6$
10 10^4	−6	0.39106641913740696600069943021	$0.112837916709556081408296703 \times 10^7$
	−7	0.39106641913741687644941720170	$0.112837916709551305629802698 \times 10^8$
	−8	0.39106641913741697555390437942	$0.112837916709551257872017758 \times 10^9$
	−9	0.39106641913741697654494925120	$0.11283791670955125739443991 \times 10^{10}$
X, No.	K	$-\mathrm{Re}\, m_{\pi/2}(\lambda = 3 + \mathrm{i}10^K)$	$\mathrm{Im}\, m_{\pi/2}(\lambda = 3 + \mathrm{i}10^K)$
	8	$0.7071067705799458684744752 \times 10^4$	$0.707106791793149304070900184 \times 10^4$
	7	$0.2236067642089612637036780 \times 10^4$	$0.223606831291000588697117346 \times 10^4$
	6	$0.7071057205269944634108438 \times 10^3$	$0.707107841847338022257921953 \times 10^3$
	5	$0.2236034436675784405393503 \times 10^3$	$0.223610151871510688350792051 \times 10^3$
	4	$0.7070007213569516578254384 \times 10^2$	$0.707212853390512126927241576 \times 10^2$
	3	$0.2232715833351843473058372 \times 10^2$	$0.223942403476875792970411256 \times 10^2$
8 6000	2	$0.6965624524541532455743379 \times 10^1$	$0.717774860127502305622301987 \times 10^1$
8 6000	1	$0.1921639059228228593918796 \times 10^1$	$0.258984680254351217840302984 \times 10^1$
10 9000	0	0.41124038393095234580849775372	$0.273042568855748993696234619 \times 10$
10 9000	−1	0.34692859559761374363143959708	$0.226163233543288726122328753 \times 10^2$
10 10^4	−2	0.34625315491557321609953557528	$0.225680708872354837170606291 \times 10^3$
10 10^4	−3	0.34624639708197048582152809498	$0.225675882173780322617849984 \times 10^4$
10 10^4	−4	0.34624632950329157372870708162	$0.225675833906649307386163053 \times 10^5$
10 10^4	−5	0.34624632882750475003190931817	$0.225675833423977982706753947 \times 10^6$
10 10^4	−6	0.34624632882074688208156817400	$0.225675833419151269458507145 \times 10^7$
	−7	0.34624632882067930339919258104	$0.225675833419103002326024534 \times 10^8$
	−8	0.34624632882067862761236882507	$0.225675833419102519654699708 \times 10^9$
	−9	0.34624632882067862085450058751	$0.22567583341910251482798645 \times 10^{10}$

Eq. (30) takes the form

$$m_0(\lambda) = \frac{C_1}{\mp 10^{-9} - \mathrm{i}10^{-9}} + \frac{C_5}{4 \mp 10^{-9} - \mathrm{i}10^{-9}} + \cdots = \frac{\mp 10^{-9} + \mathrm{i}10^{-9}}{10^{-18} - \mathrm{i}10^{-18}} C_1 + \frac{C_5}{4 - 10^{-9} - \mathrm{i}10^{-9}}. \tag{35}$$

Table 3
Values of the Titchmarsh–Weyl functions $m_0(\lambda_R + i\lambda_I)$ and $m_{\pi/2}(\lambda_R + i\lambda_I)$ for different values of λ_R and λ_I, for the case $q(x) = x^2$. The full results are analytical ones, the underlined digits show results from our numerical calculations

λ_R	λ_I	$\mathrm{Re}\, m_0(\lambda_R + i\lambda_I)$	$\mathrm{Im}\, m_0(\lambda_R + i\lambda_I)$
-1	1	0.770176746844200480445114289	0.25024384358692375419254108913
1	-1	0.381588984139117049069070137	$-1.17441835220918644394663802838$
-1	-1	0.770176746844200480445114289	$-0.25024384358692375419254108913$
1	1	0.381588984139117049069070137	1.17441835220918644394663802838
1	10^{-9}	0.391066419137416976544949251	$1.1283791670955125739443998 \times 10^9$
$1 - 10^{-9}$	10^{-9}	$5.64189583938822706037256 \times 10^8$	$5.6418958354775628699631963 \times 10^8$
$1 + 10^{-9}$	10^{-9}	$-5.64189583156689867762422 \times 10^8$	$5.6418958354775628699631963 \times 10^8$
$1 - 10^{-5}$	10^{-9}	$1.12838306647108838127843 \times 10^5$	11.2837915581654501443872355978
$1 + 10^{-5}$	10^{-9}	$-1.12837524514270561291779 \times 10^5$	11.2837915581654505448094060173
1	-10^{-9}	0.391066419137416976544949251	$-1.1283791670955125739443991 \times 10^9$
-1	10^{-9}	0.886226925452758013504748388	$3.07142847356944025113879 \times 10^{-10}$
λ_R	λ_I	$\mathrm{Re}\, m_{\pi/2}(\lambda_R + i\lambda_I)$	$\mathrm{Im}\, m_{\pi/2}(\lambda_R + i\lambda_I)$
-1	1	$-1.174418352209186443946638028$	0.38158898413911704906907013733
1	-1	$-0.250243843586923754192541089$	$-0.77017674684420048044511428946$
-1	-1	$-1.174418352209186443946638028$	$-0.38158898413911704906907013733$
1	1	$-0.250243843586923754192541089$	0.77017674684420048044511428946
3	10^{-9}	$-0.346246328820678620854500587$	$2.2567583341910251482798645 \times 10^9$
$3 - 10^{-9}$	10^{-9}	$1.12837916674926624458793 \times 10^9$	$1.1283791670955125743837056 \times 10^9$
$3 + 10^{-9}$	10^{-9}	$-1.12837916744175890222929 \times 10^9$	$1.1283791670955125743837056 \times 10^9$
$3 - 10^{-5}$	10^{-9}	$2.25675484911139921375746 \times 10^5$	22.5675831167219657431111551664
$3 + 10^{-5}$	10^{-9}	$-2.25676177403797549080729 \times 10^5$	22.5675831167219684735629683495
3	-10^{-9}	$-0.346246328820678620854500587$	$-2.2567583341910251482798645 \times 10^9$
-3	10^{-9}	$-1.772453850905516027316639623$	$2.71941230738869963276989 \times 10^{-10}$

Therefore, $\mathrm{Re}\, m_0(\lambda) \simeq \mp C_1 10^9$ and $\mathrm{Im}\, m_0(\lambda) \simeq C_1 10^9$; here we pick the dominant pole contribution. At the poles the imaginary part is dominated by the pole, and the real part is dominated by a 'background' term of Eq. (31).

In Table 3, we compare our numerical results with analytical ones. The general agreement confirms the accuracy of our results; only at very large and very small λ values does the numerical calculation show a decline in accuracy.

The numerical results throughout Table 3 obey the necessary complex conjugation property

$$m(\lambda_\mathrm{R} + \mathrm{i}\lambda_\mathrm{I}) = \overline{m}(\lambda_\mathrm{R} - \mathrm{i}\lambda_\mathrm{I}). \tag{36}$$

After making exhaustive tests for the case $q(x) = x^2$ we studied other potentials. Table 4 shows specimen $m_0(\lambda)$ function values for several forms of potential $q(x)$. Three of these have analytical solutions; besides the quoted formula for $q(x) = x^2$ we have:

(i) for $q(x) = 0$,

$$m_0(\lambda) = -\frac{\mathrm{i}}{\sqrt{\lambda}} \quad \text{for } \mathrm{Im}\,\lambda \geqslant 0 \tag{37}$$

Table 4

Comparison of some values of the Titchmarsh–Weyl function $m_0(\lambda)$ for several forms of potential as calculated by us and by other methods. For the potentials $q(x)=0,x,x^2$ the full results are analytical ones, and those with upper and lower underlining correspond to Ref. [4] and to our calculations, respectively. For the potentials $q(x)=x^3$, x^{10}, $\sin x$ the full results are our calculated results and the underlined digits are those of Ref. [4]

$q(x)$	λ_R	λ_I	Re $m_0(\lambda)$	Im $m_0(\lambda)$
	1	1	0.32179713264527913123677217	0.7768869870150186536720794
	−1	−1	−0.776886987015018653672079	0.3217971264527913123677217
0	10	10	0.1017611864088040996933812	0.2456732363513115284902715
	50	50	0.0455089860562227341304357	0.1098684113467809966039801
	100	100	0.0321797126452791312367721	0.0776886987015018653672079
	10^{-6}	10^{-6}	1.3717221641984483454429751	$1.00000188162078127149 \times 10^{-6}$
	10^{-3}	10^{-3}	1.3727211623659022261189035	$1.00188344791034295536 \times 10^{-3}$
x	1	1	0.4696702972593739875665920	1.0654819506470864134341151
	10	10	0.1017528827429881489577980	0.2469426558743188358632783
	10^{-6}	10^{-6}	1.479338721463321794138406	$1.16187126990458777817 \times 10^{-6}$
	10^{-3}	10^{-3}	1.480499426333420181009282	$1.16413881316375640513 \times 10^{-3}$
x^2	1	1	0.3815889841391170490690701	1.174418352209186443946638
	10	10	0.101452515838038047113286	0.245796385047395760930097
	1	10^{-3}	0.3910664091268632819180404	$0.112837921533569704965 \times 10^{4}$
	10^{-6}	10^{-6}	1.501316185204737536	$1.176434149957516154 \times 10^{-6}$
	10^{-3}	10^{-3}	1.502491438461537521	0.001178690677493518
x^3	1	1	0.376140361363089676	1.236863636812636230
	10	10	0.101701733899843375	0.245545371969524286
	1	10^{-3}	$0.527282613383399577 \times 10^{2}$	2.282357394677736658
	10^{-6}	10^{-6}	1.373666850619829559	$0.867606980891772141 \times 10^{-7}$
	10^{-3}	10^{-3}	1.374533587662528876	0.000868924470552375
x^{10}	1	1	0.672248823752825658	1.338682596287334186
	10	10	0.102570952567255889	0.253121181826114601
	1	10^{-3}	5.101566591730516390	0.016155822396907007
	10^{-6}	10^{-6}	1.460868872107597675	$0.129937473194902683 \times 10^{-5}$
	10^{-3}	10^{-3}	1.462166942020863048	0.001302500414846814
$\sin x$	1	1	0.453432242497456955	0.968392998820420218
	10	10	0.101769674829265222	0.246960011415918746

(ii) for $q(x)=x$,

$$m_0(\lambda)=-\frac{1}{\sqrt{\lambda}}\frac{J_{1/3}(z)+J_{-1/3}(z)}{J_{2/3}(z)-J_{-2/3}(z)},\qquad z=\frac{2}{3}\lambda^{3/2}. \tag{38}$$

Table 5 also shows results for the cases $q(x)=x^3, x^{10}, \sin x$, for various values of λ_R and λ_I. In all cases comparison is given with the method of [4] and with analytical results when available. The results suggest that the calculation can be extended with confidence to other potentials. It is important to point out that the choice of the distance X and the number of steps have played an important role in controlling the rate of convergence in our calculations. The general consideration governing our choice is that as λ increases the value of X and the number of steps both increase. To select the best converged $m_0(\lambda)$ we require stability of the results with respect to the variation

Table 5
Convergence of some $m_0(\lambda)$ for $q(x)=x^2$, for several sets of parameters X and step numbers, No. The underlined results correspond to analytic (exact) values

λ_R	λ_I	$\mathrm{Re}\, m_0(\lambda)$	$\mathrm{Im}\, m_0(\lambda)$	X, No.
		1.479338	1.16187×10^{-6}	4, 4000
10^{-6}	10^{-6}	1.4793387214	$1.161871269 \times 10^{-6}$	5, 5000
		1.47933872146332179	$1.1618712699045877 \times 10^{-6}$	8, 8000
		1.47933872146332179	$1.1618712699045877 \times 10^{-6}$	9, 9000
		1.47933872146332179413840610	$1.161871269904587778171 2 \times 10^{-6}$	
		0.3815889	1.174418	4, 4000
		0.38158898413911705	1.1744183522091864439	6, 6000
1	1	0.3815889841391170490	1.1744183522091864439	9, 9000
		0.3815889841391170490	1.1744183522091864439	$10, 10^4$
		0.381588984139117049069070 13	1.17441835220918644394663802 8	
		0.03217874	0.0776891	2, 2000
10^2	10^2	0.0321787414838014	0.0776891008204308	4, 4000
		0.03217874148380144639	0.07768910082043086631 6	6, 6000
		0.03217874148380144639	0.07768910082043086631 6	8, 8000
		0.03217874148380144639202038	0.07768910082043086631604629 0	
		0.9099338	0.5967293	4, 4000
10^{-6}	1	0.909933085104183	0.596729369127333	6, 6000
		0.90993308510418309	0.596729369127333680	9, 9000
		0.90993308510418309	0.596729369127333680	$10, 10^4$
		0.90993308510418309570813775	0.596729369127333680443653829	

of X and of the number of steps for a given λ value. This feature is made very clear in Table 5 and strengthens our confidence in the quoted results.

Even higher accuracies can be achieved at the expense of greater computation times; in general, increasing the parameter λ increases the required computation time. Because of the variable precision available, Mathematica is, of course perform codes such as the Kirby one [8] which retain a fixed double precision accuracy, although we found that the improved accuracy generally requires greater running time than that of Kirby's code for similar calculations.

The Mathematica code used in the calculations requires the input of a maximum number of allowed steps and of a specified error tolerance. It then monitors the rate of change of the solution and adjusts the step length locally throughout the integration to achieve the stated tolerance. The method used for a non-stiff problem is an implicit Adams method with an order which is internally varied up to a maximum of 12 to attain the required accuracy. Since the code is a commercial product, it is not possible for a user to access the code to reveal complete details of the technique used. In new applications, it is accordingly important to use as many test cases, comparisons with other techniques and internal consistency checks as possible. In the present application this requirement has been amply fulfilled, as the discussion indicates. Nevertheless, in view of the many works being published which use commercial packages, we wish to stress the above general guidelines about their critical application in new specialized problem areas.

6. For further reading

[13]

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